AN EXPERIMENTAL COMPARISON OF LINEAR REGRESSION METHODS USED IN MULTI-RESPONSE DESIGN PARAMETER OPTIMIZATION FOR THEIR ESTIMATION AND PREDICTION ERRORS

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submitted by **GÜLTEN GÖKAYAZ** in partial fulfillment of the requirements for the degree of **Master of Science in Industrial Engineering Department, Middle East Technical University** by,

Prof. Dr. Gülbin Dural Ünver
Dean, Graduate School of **Natural and Applied Sciences** _______________

Prof. Dr. Murat Köksalan
Head of Department, **Industrial Engineering** _______________

Prof. Dr. Gülser Köksal
Supervisor, **Industrial Engineering Dept., METU** _______________

Examining Committee Members:

Assoc. Prof. Dr. İsmail Serdar Bakal
Industrial Engineering Dept., METU _______________

Prof. Dr. Gülser Köksal
Industrial Engineering Dept., METU _______________

Assoc. Prof. Dr. Cem İyigün
Industrial Engineering Dept., METU _______________

Assoc. Prof. Dr. Ceylan Talu Yozgatlıgil
Statistics Dept., METU _______________

Assist. Prof. Dr. Özlem Türker Bayrak
Statistics Dept., Çankaya University _______________

Date: July 27, 2016

I hereby declare that all information in this document has been obtained and presented in accordance with academic rules and ethical conduct. I also declare that, as required by these rules and conduct, I have fully cited and referenced all material and results that are not original to this work.

Name, Last Name: GÜLTEN GÖKAYAZ

Signature:

ABSTRACT

AN EXPERIMENTAL COMPARISON OF LINEAR REGRESSION METHODS USED IN MULTI-RESPONSE DESIGN PARAMETER OPTIMIZATION FOR THEIR ESTIMATION AND PREDICTION ERRORS

Gökayaz, Gülten

M.S., Department of Industrial Engineering

Supervisor: Prof. Dr. Gülser Köksal

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Product and process designers need to find most preferable settings of design parameters to simultaneously achieve multiple quality objectives based on some performance measures such as means and variances of quality characteristics. In these optimization studies, typically empirical models of such performance measures are utilized. These models are usually developed based on data collected through statistically designed experiments using linear regression methods such as Ordinary Least Squares (OLS), Weighted Least Squares (WLS), and Seemingly Unrelated Regression (SUR). In multi-response design parameter optimization (MRDPO) problems, it is assumed that each response has a non-homogeneous variance. Furthermore, responses might be correlated. These linear regression methods might not be appropriate for a particular MRDPO problem due to their restrictive assumptions. Hence, estimation errors associated with model parameters and prediction errors associated with individual observations might be large depending on the problem situation. In this study, we are interested in examining and comparing these errors on a typical MRDPO problem with two responses under different scenarios systematically generated by statistical design of experiments. In addition, we develop a bootstrapping approach to compute joint confidence and prediction regions for estimated mean responses and individual observations, respectively, since these regions are not analytically available for some methods. Our observations based on analysis of experimental results using certain performance measures and graphs of the confidence and prediction regions are presented. Concluding remarks are given and future studies are recommended for generalization of these observations.

Keywords: multi-response design parameter optimization, linear regression, heteroscedasticity, correlated responses, bootstrap confidence and prediction regions.

ÖZ

ÇOK YANITLI TASARIM PARAMETRE OPTİMİZASYONU İÇİN KULLANILAN DOĞRUSAL REGRESYON YÖNTEMLERİNİN TAHMİN VE ÖNGÖRÜ HATASI BAKIMINDAN DENEYSEL KARŞILAŞTIRMASI

Gökayaz, Gülten

Yüksek Lisans Endüstri Mühendisliği Bölümü

Tez Yöneticisi: Prof. Dr. Gülser Köksal

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Tasarım parametre optimizasyonu, bir ürün ya da sürecin kalitesini iyileştirmek için kullanılan bir kalite mühendisliği yaklaşımıdır. Bu problemde amaç, kontrol edilebilen ürün ve süreç parametrelerinin, kontrol edilemeyen faktörlerin değişkenliği artırıcı etkisine rağmen, hedeflenen kalite performansını istikrarlı bir şekilde sağlayacak en iyi seviyelerini belirlemektir. Bu optimizasyon çalışmalarında, istatistiksel olarak tasarlanmış deneylerden toplanan veriler kullanılarak tanımlanan kalite karakteristiği için ortalama değer ve varyans gibi performans ölçüleri ile tasarım parametreleri arasındaki ilişki ampirik olarak modellenir. Bu modeller genellikle en küçük kareler (OLS), ağırlıklı en küçük kareler (WLS) ve görünürde ilişkisiz regresyon (SUR) gibi doğrusal regresyon yöntemleri kullanılarak elde edilmektedir. Çok yanıtlı tasarım parametre optimizasyon (ÇYTPO) problemlerinde, her yanıt için farklı deney noktalarında varyansın sabit (homojen) olmadığı varsayılır. Ayrıca, yanıtların birbiriyle ilişkili olması söz konusu olabilir. Bahsedilen doğrusal regresyon yöntemleri, sahip oldukları kısıtlayıcı varsayımlar sebebiyle belli bir ÇYTPO problemi için uygun olmayabilir. Dolayısıyla model parametreleri ve belli noktalarda yapılan ortalama değer tahmini ve tek bir gözlem için yapılan öngörüdeki hatalar duruma bağlı olarak büyük olabilir. Bu çalışmada, iki yanıtlı tipik bir ÇYTPO problemi ele alınıp, istatistiksel deney tasarımı ile sistematik olarak oluşturulan farklı senaryolar altında bahsedilen doğrusal regresyon yöntemleri incelenmiş ve karşılaştırılmıştır. Bu çalışmada ayrıca özyükleme yöntemi kullanılarak belli noktalarda, ortalama değer ve tek bir gözlemin değeri için, sırasıyla, güven ve tahmin bölgeleri elde edilmiştir. Son olarak, yapılan gözlemler paylaşılmış ve bu gözlemlerin genelleştirilebilmesi için gelecekte yapılabilecek çalışmalar hakkında öneriler verilmiştir.

Anahtar Kelimeler: çok yanıtlı tasarım parametre optimizasyonu, doğrusal regresyon, değişen varyans, ilişkili yanıtlar, özyükleme güven ve tahmin bölgeleri

To my family

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LIST OF ABBREVIATIONS

RPD	Robust Parameter Design
DPO	Design Parameter Optimization
RSM	Response Surface Methodology
MRDPO	Multi-Response Design Parameter Optimization
MRSO	Multi-Response Surface Optimization
OLS	Ordinary Least Squares
GLS	Generalized Least Squares
WLS	Weighted Least Squares
MVR	Multivariate Regression
SUR	Seemingly Unrelated Regression
MSE	Mean Square Error
BLUE	Best Linear Unbiased Estimator

CHAPTER 1

INTRODUCTION

Robust parameter design (RPD) or design parameter optimization (DPO) is a methodology widely used in quality engineering to improve the quality of products and processes. Using this methodology, settings (nominal or target values) of controllable product and process design parameters are determined to consistently achieve target quality performance subject to the effects of uncontrollable factors. RPD was defined by a Japanese engineer, Genichi Taguchi in the 1950s, and it has been widely used by industrial organizations since 1980s. Taguchi proposed some solution methods to the RPD problems based on statistical design and analysis of experiments, which brought about many criticisms and discussions. Following these criticisms, many research studies have been conducted on the RPD problem and many alternative approaches have been developed. The review paper by Robinson et al. [1] gives some important aspects of the RPD problem, the criticisms to Taguchi's method and works that have addressed them since 1992. Park et al. [2] also give an overview of RPD problem and classify the RPD methods into three categories: The Taguchi method, robust optimization, and robust design with the axiomatic approach; then, they analyze these methods from both theoretical and application viewpoints.

One widely used methodology for the RPD problems is the response surface methodology (RSM). It utilizes both mathematical and statistical techniques and is employed in basically three steps: Screening, modeling and optimization [3]. Screening step includes identifying the quality characteristic of interest and controllable factors affecting it. In the modeling step, the true relationship between the response and controllable factors, which is unknown, is approximated by a low-degree polynomial model. Experiments are designed in order to collect data and presumed model is fitted to the experimental data. At the final step, some optimization techniques are applied to the empirical model in order to find the optimal levels of the controllable factors over the region of interest.

RSM approach traditionally considers a single response, i.e. a single quality characteristic. However, quality of a product or a process is naturally defined by more than one response, and these are most likely correlated. In such a case, multiple responses should be optimized simultaneously. This problem is called as multi-response design parameter optimization (MRDPO) problem, which is a multi-response surface optimization (MRSO) problem [4].

According to Costa and Pereira [3], multi-response surface optimization approaches can be classified into desirability function-based optimization, loss function-based optimization and generalized distance function-based optimization. These are all based on converting the multi-response problem into a single response problem. However, there are other methods handling the multi-response problem in different ways. Lee at al. [4] address the MRSO methods with the viewpoint of multi-objective decision making and provide a broader classification for them.

Regardless of the optimization approach used, response surface models need to be fit to performance measures such as mean, variance and correlation corresponding to each quality characteristic. In our study, we put emphasis on modeling mean responses. To obtain accurate models is quite important. Otherwise, selected operating levels may not result in desired and expected performance.

Using collected data through statistically designed experiments, the parameters in the response surface models are usually estimated by ordinary least squares (OLS) method. One of the underlying assumptions of OLS is that the response has a constant variance at different design variable settings. However, this assumption is against the nature of the parameter design problems which are formulated and solved assuming that there exists a solution where the variance is minimal. In the case that the variance of the response differs according to the design variable setting, i.e. heteroscedasticity, some variance-stabilizing transformations may be used before applying OLS. However, finding an appropriate transformation may not be easy or possible. Furthermore, after fitting linear models to the transformed response variables, estimating the responses in their original scales is not easy [5].

In the existence of both heteroscedasticity and correlation between observations of a response at different design variable settings, i.e. serial correlation or autocorrelation, generalized least squares (GLS) can be used to estimate the model parameters. In the parameter design problems, serial correlation is not usually expected, since the run sequence in the experiments is randomized. However, as it has previously been pointed out, it is quite expected to have non-homogeneous variances at different design variable settings. Then, weighted least squares (WLS), a special case of GLS, can be put in use.

OLS, WLS and GLS regression techniques consider multiple responses separately. However, when there is more than one mean response to consider, a better practice is to build the empirical models simultaneously, especially if the responses are correlated. Multivariate regression (MVR) and seemingly unrelated regression (SUR) are methods that consider this correlation. However, they do not take the heteroscedasticity into account. There are some studies that consider heteroscedasticity in SUR such as Mandy and Martins-Filho [6]. However, they consider only certain types of heteroscedasticity. There are also some methods in time series literature such as vector autoregression which considers a general variance-covariance structure. However, they have not been adopted for use in MRDPO problems yet, to the best of our knowledge. Hence, these methods are left out of the scope of our study.

In the statistics literature, linear regression methods mainly consist of OLS and MVR. They rarely cover WLS and GLS, and almost never cover SUR. However, in the context of robust parameter design, we observe an increasing interest of researchers in WLS and SUR. Ko et al. [7] use SUR in some cases of their study. Shah et al. [8] show that SUR estimates responses more precisely than OLS, if the responses are correlated. Fogliatto and Albin [9] give a regression tutorial including

OLS, GLS, MVR and SUR. However, none of these studies make a comprehensive comparison of these methods in terms of their estimation and prediction errors.

MRDPO researchers and practitioners need empirical model building approaches that allow them to build models of performance measures with high accuracy and precision under heterocedasticity, and in some cases, correlated multiple responses. They seem to choose one of the linear regression methods such as OLS, WLS and SUR without knowing much about how much model uncertainty the chosen method introduces to the design parameter optimization problem.

In this study, we are interested in examining and comparing the accuracy and precision of the linear regression methods typically used in formulating and solving MRDPO problems. The purpose of our study is to give an idea about magnitudes of model parameter uncertainty levels of these linear regression methods. Our comparison approach is experimental in the sense that it considers a typical MRDPO problem and makes observations based on several cases of this problem. The problem has two responses of which the true models and error distributions are known. The cases or scenarios are systematically generated by statistical design of experiments considering the following factors: number of replications, error variance homogeneity, correlation between responses and position of the design point. The response surface models use the same set of predictors, but certain methods are also compared allowing different sets of response predictors. For each scenario a data set is generated using simulation. Then, confidence regions of expected responses and prediction regions of future observations at different design parameter points are computed separately for each linear regression method using bootstrapping. Finally, observations are made about differences among the linear regression methods in magnitudes of estimation and prediction errors.

The complexity in the application of the methods mentioned so far, apart from the OLS, is due to the lack of information about the values of the variances of the responses and the correlations among them. However, in order to obtain accurate models for the mean responses, we need to use information regarding the variance-covariance matrix, which is most probably unknown and needs to be estimated. Generalized linear models, maximum likelihood estimators are some methods used in this manner. In our study, however, we leave the variance and correlation estimation out of scope. We simply use sample variances while applying WLS. In order to apply SUR, we estimate the variance-covariance matrix based on the OLS residuals as Zellner [10], who developed SUR, suggests. Still, to exclude the effect of the accuracy in the estimation of variance-covariance matrix on the performances of the methods, we also make analyses under the assumption that variance-covariance matrix of the mean responses is known.

The performance measures used in the comparison are coefficient of determination (R^2), mean square error (MSE), some measures related to the prediction variance of unknown parameters, variances of the predicted mean responses at certain design settings, Hellinger distance between true and predicted distributions of a single observation defined at certain design settings. Besides, we provide joint confidence and prediction regions for the estimated mean responses by using a bootstrap technique.

The organization of the thesis is as follows: In Chapter 2, we give background information on design parameter optimization problem. Then, we introduce the model parameter estimation methods such as OLS, GLS, WLS, MVR and SUR in the context of RSM. Then, we define the accuracy measures used to compare these methods. Also, we provide a review on constructing the joint confidence and prediction regions by a bootstrap technique. In Chapter 3, we define the scenarios generated to evaluate the performances of the methods. Besides, a detailed explanation about how the regression methods and the bootstrap technique are applied is given. In Chapter 4, we show the computational results and provide a discussion about them. In Chapter 5, we provide concluding remarks and define possible future studies.

CHAPTER 2

LITERATURE REVIEW

In this section, we first give background information on the design parameter optimization problem. Then, we present the parameter estimation methods OLS, GLS, WLS, MVR and SUR in the context of RSM. Then, we define the performance measures used in comparison of these methods. Also, we provide a review on constructing the joint confidence and prediction regions by a bootstrap technique.

2.1 Robust Parameter Design Problems

RPD is a quality engineering methodology applied to improve the quality of the products and processes at the design stage. The idea is to determine the design parameters of the products and/or the processes so as to make them robust to uncontrollable sources of variation. The objective, meanwhile, is to minimize quality costs.

RPD is first described by the Japanese engineer, Genichi Taguchi in the 1950s. Taguchi classifies the factors as controllable (design) factors and uncontrollable (noise) factors. The controllable factors are easily controlled by the designer while the uncontrollable factors are not. Accordingly, Taguchi suggests determining the levels of controllable factors in a way to achieve robustness on the response despite the existence of noise factors. He represents robustness by the quality loss function [2] which is

$$\mathrm{L}(y) = b(y - t)^2 \tag{2.1}$$

where b is loss coefficient, y is the response, and t is the target value for the response. The loss, here, is considered as the cost incurred by the society due to the difference between the response and its target value. Derived from (2.1), the expected value of the loss function is

$$\mathrm{E}[\mathrm{L}(y)] = b[\sigma^2 + (\mu - t)^2] \tag{2.2}$$

where μ and σ^2 are the mean and the variance of y, respectively.

As can be seen in (2.2), the expected loss function has two components: variance (σ^2) and square of the mean's deviation from the target. In order to minimize the expected loss function, Taguchi proposes a two-step procedure. In the first step, the variability in response is minimized while, in the second step, the mean value is brought to the target as much as possible. Taguchi employs the crossed designs for RPD experiments and proposes the use of signal-to-noise ratio, SNR which is a criterion maximized to come up with the optimal product and process parameter settings.

Robinson et al. [1] summarize Taguchi's contributions to robust parameter design into three areas: Quality philosophy, experimental design and data analysis. They point out that although Taguchi's quality philosophy gains acceptance and appreciation, his experimental design and data analysis are subjects of many criticisms. Most of the references related to RPD give an extensive coverage of these criticisms. Nair [11], Myers et al. [12], Khuri and Mukhopadhyay [13] and Montgomery [14] are among the references which discuss Taguchi's methodology in detail. As Park et al. [2] do, it is possible to itemize the critics as follows: 1) Interactions among the controllable factors cannot be estimated through the design of experiment suggested by Taguchi. 2) The design of experiment is not efficient in terms of the number of experimental runs. 3) SNR is effective only in the cases where it is possible to distinguish the controllable factors affecting the mean from those affecting the variance. 4) Taguchi provides a solution methodology to handle a single quality characteristic.

Following the criticisms of Taguchi's work, many research studies have been conducted on the RPD problem and many alternative approaches have been developed. The most popular approaches are based on the RSM. It was first introduced by [15], and it utilizes both mathematical and statistical techniques to solve many different industrial problems including RPD [16].

Costa and Pereira [3] define three general phases in the RSM: Screening, modeling and optimization. In the screening phase, an experiment is designed to identify the significant controllable factors to the response of interest. In the modeling phase, the true relationship between the response and controllable factors, which is unknown, is approximated by a low-degree polynomial model. Most frequently, a first-order or second-order model is used. Designing another experiment at this phase, the presumed model is fitted to the experimental data. At the final phase, some optimization techniques are applied to the empirical model in order to find the optimal levels of the factors over the region of interest.

There are two RSM approaches to the RPD introduced in the 1990s: Single response approach and dual model approach. In the former approach, there are two separate response surface models for the mean and the variance. However, the mean surface model is first built including both controllable and uncontrollable variables, and then the variance model is obtained from the mean's model theoretically. In the latter approach, again there are two response models: one for the mean and one for the variance. However, these models are fitted separately and empirically, also including only the controllable factors [13]. Afterwards, the optimal levels of controllable factors are determined by optimizing the primary response subject to the secondary response. Even though which response to be the primary is the decision of the designer, considering the Taguchi's RPD philosophy, the primary response is generally taken as the variance and it is minimized while the secondary response is defined as the mean and it is forced to be on the target. An extensive knowledge of the theory and the application of the RSM can be achieved through Box and Draper [16], Myers and Montgomery [17], Khuri and Cornell [18].

Besides, there are some review papers on RSM such as Myers et al. [19], Khuri and Mukhopadhyay [13].

The traditional RSM approach handles a single response, i.e. a single quality characteristic. However, quality of a product or a process is naturally defined by more than one response, and these are most likely to be correlated. In such a case, finding the optimal levels of controllable variables for each response separately cannot be a good approach since improvement in one response may result in a worsening of another one. The problem of finding optimal levels of controllable factors by considering the multiple responses simultaneously is called multi-response design parameter optimization or multi-response surface optimization problem.

According to Costa and Pereira [3], multi-response optimization approaches can be classified into desirability function-based optimization, loss function-based optimization and generalized distance function-based optimization.

Desirability function approach is first introduced by Harrington [20] and then modified by Derringer and Suich [21]. The method basically converts each estimated response to a desirability value depending on the type of the quality characteristic. The operating conditions are determined by maximizing overall desirability which is the geometric mean of the individual desirability values. The main drawback of the method is that it totally ignores the variance-covariance structure of the responses.

Loss function approach in multi-response context is originated from the Taguchi's univariate loss function. This approach aims to determine the optimal operating conditions by minimizing an expected loss. There are several methods using the loss function approach in the literature including Pignatiello [22], Vining [23] and Ko et al. [7]. Ko et al. [7] define three desirable properties: Small bias (small deviation of a response from its target), high robustness (small variance of true response), and high quality of predictions (small variance of the predicted responses). Accordingly, the existing methods define the expected loss considering some or all of these properties. The advantages of loss function approach are that the variance-covariance structures of the responses and the process economics are taken into account. However, representing the process economics is not straightforward.

Khuri and Conlon [24] suggested a generalized distance function-based optimization. It is a special case of loss functions. The advantage of their method is that it considers the correlation between responses and the quality of the predictions. However, it requires all responses to be modeled by the same set of control factors. Also, it considers neither the preferences of the decision maker nor the economic implications of the process.

The classification made by Costa and Pereira [3] seems to consider MRSO approaches most frequently used in the literature. These are all based on converting the multi-response problem into a single response problem. For a more detailed classification, Lee at al. [4] can be used. They address the MRSO methods with the viewpoint of multi-objective decision making and provide a broader classification for them.

No matter which optimization technique is used, response surface models need to be fit to the performance measures (mean, variance, correlation and so on) corresponding to each quality characteristic. In our study, we put emphasis on modeling mean responses. To obtain accurate models is quite important. Ouyang et al. [25] illustrate the importance of model uncertainty on the true performance of the system with the help of Figure 2.1. In this figure, true model is unknown and approximated by the empirical model. Considering that the aim is to maximize the performance response, result of the optimization will be point B. However, at point B, the true performance is quite low. On the other hand, the performance of the true optimal point, which is A, seems to be very low according to the empirical model. Thus, in order to get closer to the optimal performance, the accuracy of the empirical model should be high or somehow the error in the empirical model should be taken into account in the optimization. In order to increase the accuracy of the estimation, we search for alternative regression methods. Also, we provide confidence and prediction regions for the estimated response so that the designer can determine the optimal design setting considering the accuracy at the corresponding point.

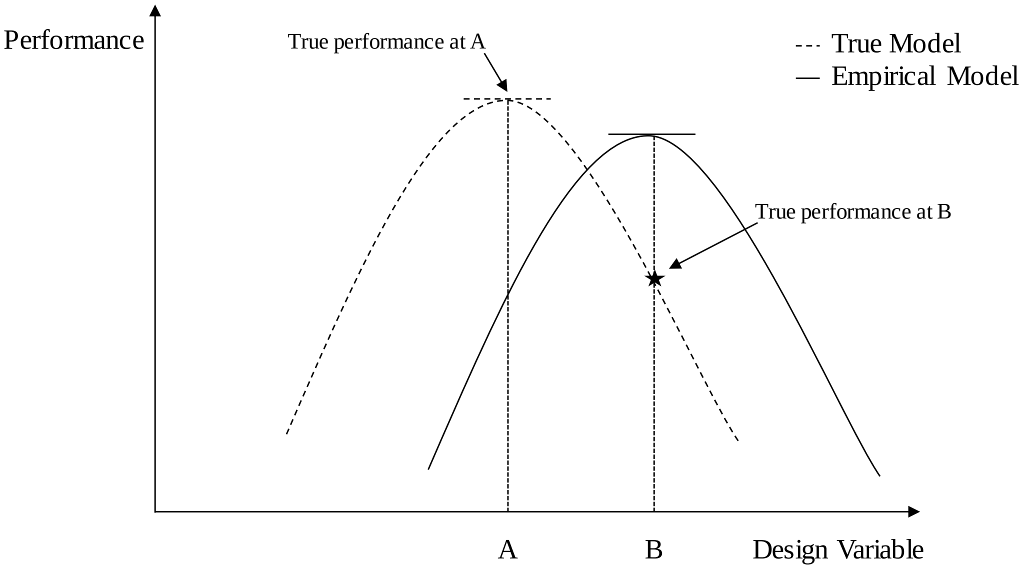

Figure 2.1 Error in process optimization due to model uncertainty [25]

However, in order to obtain accurate models for the mean responses, we need to use information regarding the variance-covariance matrix of them, which is most probably unknown and needs to be estimated. Still, we leave the estimation of the variance-covariance matrix out of our scope. We simply use sample variances while applying WLS. In order to apply SUR, we estimate the variance-covariance matrix based on the OLS residuals as Zellner [10], who developed SUR, suggests.

2.2 Parameter Estimation in a Multi-Response System

In RSM, the functional relationship between a response (y) and a set of controllable variables ($x_1, x_2, \ldots, x_r$) is approximated by a low-degree polynomial model. Mostly, a second-order model is used. The second order model is expressed as

$$y = \beta_0 + \sum_{i=1}^{r} \beta_i x_i + \sum_{i=1}^{r} \beta_{ii} x_i^2 + \sum_{i<k} \sum_{k=2}^{r} \beta_{ik} x_i x_k + \varepsilon \qquad (2.3)$$

where β's are unknown parameters and ε is a random error.

The unknown parameters β's in (2.3) are estimated using collected data through statistically designed experiments. Suppose that there are n observations. Then, for each observation $y_{(j)}$, the model given in (2.3) is written as follows:

$$y_{(j)} = \beta_0 + \sum_{i=1}^{r} \beta_i x_{i(j)} + \sum_{i=1}^{r} \beta_{ii} x_{i(j)}^2 + \sum_{i<k} \sum_{k=2}^{r} \beta_{ik} x_{i(j)} x_{k(j)} + \varepsilon_{(j)} \qquad (2.4)$$

where $j = 1, 2, \ldots, n$

The set of linear equations in (2.4) can be expressed in matrix notation.

$$\mathbf{y} = \mathbf{X\beta} + \boldsymbol{\varepsilon} \qquad (2.5)$$

$$\text{where } \mathbf{y} = \begin{bmatrix} y_{(1)} \\ y_{(2)} \\ \vdots \\ y_{(n)} \end{bmatrix}, \qquad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_r \\ \beta_{11} \\ \vdots \\ \beta_{rr} \\ \beta_{12} \\ \vdots \\ \beta_{r-1\,r} \end{bmatrix}, \qquad \boldsymbol{\varepsilon} = \begin{bmatrix} \varepsilon_{(1)} \\ \varepsilon_{(2)} \\ \vdots \\ \varepsilon_{(n)} \end{bmatrix}$$

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1(1)} & \cdots & x_{r(1)} & x_{1(1)}^2 & \cdots & x_{r(1)}^2 & x_{1(1)}x_{2(1)} & \cdots & x_{r-1(1)}x_{r(1)} \\ 1 & x_{1(2)} & \cdots & x_{r(2)} & x_{1(2)}^2 & \cdots & x_{r(2)}^2 & x_{1(2)}x_{2(2)} & \cdots & x_{r-1(2)}x_{r(2)} \\ & & & & & & \vdots & & & \\ 1 & x_{1(n)} & \cdots & x_{r(n)} & x_{1(n)}^2 & \cdots & x_{r(n)}^2 & x_{1(n)}x_{2(n)} & \cdots & x_{r-1(n)}x_{r(n)} \end{bmatrix}$$

The response surface modeling problem described so far includes a single response, i.e. a single quality characteristic. However, quality of a product or a process is naturally defined by more than one response. Then, for each response, a model, say the model given in (2.3), needs to be fit. Considering an experiment with m responses $y_1, y_2, \ldots y_\mathrm{m}$ and n observations on each response, the set of linear equations for the i^{th} response in matrix notation is

$$\mathbf{y}_i = \mathbf{X}_i\boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i \quad i = 1,2, \ldots, m \tag{2.6}$$

Equation (2.6) is equivalent to equation (2.5) written for each response. Accordingly, two approaches can be adopted to obtain unknown parameters in each response model. The first approach requires modeling each response individually. OLS, WLS and GLS are regression techniques that consider the responses separately. In the second approach, the models of the responses are built simultaneously. This approach gains importance especially when there is correlation between responses. MVR and SUR are techniques that fit models to the responses at the same time [9].

2.2.1 Ordinary Least Squares

OLS is a widely used method in order to estimate unknown parameters in (2.5). In OLS regression, ε is assumed to be distributed independently and normally with a mean 0 and constant variance σ^2 for any set of $x_1, x_2, \ldots, x_r$. One can denote this as follows:

$$\boldsymbol{\varepsilon} \sim \mathbf{N}(\mathbf{0}, \sigma^2\mathbf{I}_n)$$

where $\mathbf{I}_n$ is an $n \times n$ identity matrix.

OLS determines estimates of the model parameters by minimizing the sums of the squares of the errors:

$$\text{Min } \boldsymbol{\varepsilon}'\boldsymbol{\varepsilon} = \sum_{j=1}^{n} \varepsilon_{(j)}^2$$

The OLS estimator of $\boldsymbol{\beta}$ is obtained by

$$\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$$

Accordingly, the fitted values and the residuals are as given by the following equations:

$$\hat{\mathbf{y}}_{\mathbf{OLS}} = \mathbf{X}\,\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}$$

$$\hat{\boldsymbol{\varepsilon}}_{\mathbf{OLS}} = \mathbf{y} - \hat{\mathbf{y}}_{\mathbf{OLS}}$$

The OLS estimator shows the following properties:

$$\begin{aligned}\mathbf{E}[\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}] &= \mathbf{E}[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}] = \mathbf{E}[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon})] \\ &= \mathbf{E}[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\varepsilon}] = \boldsymbol{\beta}\end{aligned}$$

$$\begin{aligned}\mathbf{Cov}\left(\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}\right) &= \mathbf{Var}\left(\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}\right) = \mathbf{Var}[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}] \\ &= (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Var}(\mathbf{y})[(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}']' = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1} \\ &= \sigma^2(\mathbf{X}'\mathbf{X})^{-1}\end{aligned}$$

Then,

$$\widehat{\boldsymbol{\beta}}_{\mathrm{OLS}} \sim \mathrm{N}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}'\mathbf{X})^{-1})$$

Note that σ^2 is generally unknown and the mean square error (MSE) is used as an unbiased estimator of it.

$$\hat{\sigma}^2 = \mathrm{MSE} = \frac{\mathrm{SSE}}{n - (\text{number of estimated } \beta \text{ parameters})}$$

where SSE is the sum of square error, i.e. $\mathrm{SSE} = \hat{\boldsymbol{\varepsilon}}_{\mathbf{OLS}}{}'\hat{\boldsymbol{\varepsilon}}_{\mathbf{OLS}}$

According to the Gauss-Markov theorem, the OLS estimators are the best (minimum variance) linear unbiased estimators (BLUE) of unknown parameters when the underlying assumptions are valid [5]. However, in the design parameter optimization problems, the constant variance assumption does not make sense because these problems are formulated and solved assuming that there exists a solution where the variance is minimal.

Let Var($\boldsymbol{\varepsilon}$) =$\sigma^2\mathbf{V}$ so that $\mathbf{V} \neq \mathbf{I}_n$. Then,

$$\mathbf{E}[\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}] = \boldsymbol{\beta}$$

$$\begin{aligned}\mathbf{Cov}(\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}) = \ &\mathbf{Var}(\widehat{\boldsymbol{\beta}}_{\mathbf{OLS}}) = \mathbf{Var}[(\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\mathbf{X}'\mathbf{y}] \\ &= (\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\mathbf{X}'\mathbf{Var}(\mathbf{y})[(\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\mathbf{X}']'\end{aligned}$$

$$= \sigma^2(\mathbf{X}'\mathbf{X})^{-\mathbf{1}}\mathbf{X}'\mathbf{V}\mathbf{X}(\mathbf{X}'\mathbf{X})^{-\mathbf{1}} \text{ [5]}$$

In such a case, the OLS estimator is still unbiased, but its BLUE property is not valid any more. It means that the standard errors of the estimated parameters are unnecessarily larger. Still, in practice, OLS is widely used and generally some variance-stabilizing transformations are made before applying OLS. However, transformations may not work to solve the problem. Besides, it takes time and needs expertise. Moreover, after fitting models to the transformed variables, it is not straightforward to turn back to the original scale. Direct inverse transformation does not always give the mean of the response. Confidence and prediction intervals can be transformed to the original scale by applying direct inverse operation since the percentiles are not affected by any transformation. Still, the resulting intervals in the original scale may not be the shortest [5]. There are some studies which suggest procedures to obtain unbiased point estimates for some transformations such as Neyman and Scott [26], Miller [27], Shen and Zhu [28]. However, in the scope of this study, we are interested in the alternative modeling approaches that deal with the deficiencies in OLS directly.

2.2.2 Generalized Least Squares and Weighted Least Squares

Concerning the model in (2.5), GLS assumes a more general variance-covariance matrix for the error terms, that is

$$\boldsymbol{\varepsilon} \sim \mathbf{N}_n(\mathbf{0}, \sigma^2\mathbf{V})$$

where $\mathbf{V}$ is a known, positive definite $n \times n$ matrix. If $\mathbf{V}$ is the identity matrix ($\mathbf{V} = \mathbf{I}$), GLS and OLS are equivalent. Otherwise, GLS is capable of producing more efficient estimators. If $\mathbf{V}$ has off-diagonal elements rather than zero, it means that error terms at different design settings are correlated, i.e. serial correlation or autocorrelation exists. However, in the RPD problems, serial correlation is not expected since the run sequence in the experiments is randomized. Still, as previously pointed out, it is quite expected to have non-homogeneous variances at different design settings, i.e. heteroscedastic errors. In this case, $\mathbf{V}$ can be considered as a diagonal matrix the diagonal elements of which are not equal. Then, the regression technique is called WLS. Although WLS is a special case of GLS, in our study they will be referred to as the same. Let $\mathbf{V}$ have the following form:

$$\mathbf{V} = \begin{bmatrix} 1/w_1 & 0 & \cdots & 0 \\ 0 & 1/w_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \cdots & 1/w_n \end{bmatrix}$$

WLS determines the estimates of the model parameters by minimizing the weighted sums of the squares of the errors which is

$$\text{Min } \boldsymbol{\varepsilon}'\mathbf{V}^{-1}\boldsymbol{\varepsilon} = \sum_{j=1}^{n} w_i \varepsilon_{(j)}^2$$

WLS gives weights to each observation so that observations with large variances have less influence in determining the model parameters while the observations with small variances have more. By giving weights to the observations, the original model is actually transformed so that OLS assumptions are valid, and hence OLS is applicable. Since $\mathbf{V}$ is a positive definite matrix, there exists a nonsingular matrix $\mathbf{P}$ such that $\mathbf{P}'\mathbf{P} = \mathbf{V}$. Then, premultiplying the original model in (2.5) by $\mathbf{P}^{-1}$, we obtain:

$$\mathbf{P}^{-1}\mathbf{y} = \mathbf{P}^{-1}\mathbf{X}\boldsymbol{\beta} + \mathbf{P}^{-1}\boldsymbol{\varepsilon}$$

$$\mathbf{y}^* = \mathbf{X}^*\boldsymbol{\beta} + \boldsymbol{\varepsilon}^* \tag{2.7}$$

Then,

$\mathrm{E}(\boldsymbol{\varepsilon}^*) = \mathrm{E}(\mathbf{P}^{-1}\boldsymbol{\varepsilon}) = \mathbf{0}$

$$\begin{aligned}\mathrm{Cov}(\boldsymbol{\varepsilon}^*) &= \mathrm{Cov}(\mathbf{P}^{-1}\boldsymbol{\varepsilon}) = \mathbf{P}^{-1}\mathrm{Cov}(\boldsymbol{\varepsilon})(\mathbf{P}^{-1})' = \sigma^2\mathbf{P}^{-1}\mathbf{V}(\mathbf{P}^{-1})' \\ &= \sigma^2\mathbf{P}^{-1}\mathbf{P}\mathbf{P}'(\mathbf{P}^{-1})' = \sigma^2\mathbf{I}\end{aligned}$$

Applying OLS to the transformed model, WLS estimators are obtained by

$$\widehat{\boldsymbol{\beta}}_{\mathrm{WLS}} = (\mathbf{X}^{*\prime}\mathbf{X}^*)^{-1}\mathbf{X}^{*\prime}\mathbf{y}^* = (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}$$

Accordingly, the fitted values and the residuals are

$$\hat{\mathbf{y}}_{\mathbf{WLS}} = \mathbf{X}\,\widehat{\boldsymbol{\beta}}_{\mathbf{WLS}}$$

$$\hat{\boldsymbol{\varepsilon}}_{\mathbf{WLS}} = \mathbf{y} - \hat{\mathbf{y}}_{\mathbf{WLS}}$$

The WLS estimator shows the following properties:

$$\begin{aligned}\mathrm{E}\big[\widehat{\boldsymbol{\beta}}_{\mathrm{WLS}}\big] &= \mathrm{E}[(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}] = \mathrm{E}[(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon})] \\ &= \mathrm{E}[(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\boldsymbol{\varepsilon}] = \boldsymbol{\beta}\end{aligned}$$

$$\begin{aligned}\mathbf{Cov}\big(\widehat{\boldsymbol{\beta}}_{\mathbf{WLS}}\big) &= \mathbf{Var}\big(\widehat{\boldsymbol{\beta}}_{\mathbf{WLS}}\big) = \mathbf{Var}[(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{y}] \\ &= (\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{Var}(\mathbf{y})[(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}]' \\ &= \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'\mathbf{V}^{-1}\mathbf{V}[(\mathbf{V}')^{-1}\mathbf{X}(\mathbf{X}'(\mathbf{V}')^{-1}\mathbf{X})^{-1}] = \\ &= \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\mathbf{X}'(\mathbf{V}')^{-1}\mathbf{X}(\mathbf{X}'(\mathbf{V}')^{-1}\mathbf{X})^{-1} = \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\end{aligned}$$

or basically,

$$\begin{aligned}\mathbf{Cov}\big(\widehat{\boldsymbol{\beta}}_{\mathbf{WLS}}\big) &= \sigma^2(\mathbf{X}^{*\prime}\mathbf{X}^*)^{-1} = \sigma^2((\mathbf{P}^{-1}\mathbf{X})'\mathbf{P}^{-1}\mathbf{X})^{-1} = \sigma^2(\mathbf{X}'(\mathbf{P}')^{-1}\mathbf{P}^{-1}\mathbf{X})^{-1} \\ &= \sigma^2(\mathbf{X}'(\mathbf{P}'\mathbf{P})^{-1}\mathbf{X})^{-1} = \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1}\end{aligned}$$

Then,

$$\widehat{\boldsymbol{\beta}}_{\mathrm{WLS}} \sim \mathrm{N}(\boldsymbol{\beta}, \sigma^2(\mathbf{X}'\mathbf{V}^{-1}\mathbf{X})^{-1})$$

Residuals for the transformed model (2.7) are

$$\tilde{\boldsymbol{\varepsilon}}_{\mathbf{WLS}} = \mathbf{V}^{-\frac{1}{2}}(\mathbf{y} - \hat{\mathbf{y}}_{\mathbf{WLS}})$$

The mean square error obtained from the transformed model is an unbiased estimator of σ^2

$$\hat{\sigma}^2 = \mathrm{MSE_{WLS}} = \frac{\mathrm{SSE_{WLS}}}{n - (\text{number of estimated } \beta \text{ parameters})}$$

where $\mathrm{SSE_{WLS}}$ is the sum of square error such that

$$\mathrm{SSE_{WLS}} = \tilde{\boldsymbol{\varepsilon}}_{\mathbf{WLS}}{}' \tilde{\boldsymbol{\varepsilon}}_{\mathbf{WLS}} = \hat{\boldsymbol{\varepsilon}}'_{\mathbf{WLS}} \mathbf{V}^{-1} \hat{\boldsymbol{\varepsilon}}_{\mathbf{WLS}}$$

Once the matrix **V** is known, $\widehat{\boldsymbol{\beta}}_{\mathrm{WLS}}$ is the BLUE of **β**. However, in practice, **V** is unknown and need to be estimated. Then, the method is called feasible WLS, and the model parameter estimator is obtained as

$$\widehat{\boldsymbol{\beta}}_{\mathrm{FWLS}} = \left(\mathbf{X}'\widehat{\mathbf{V}}^{-\mathbf{1}}\mathbf{X}\right)^{-\mathbf{1}}\mathbf{X}'\widehat{\mathbf{V}}^{-\mathbf{1}}\mathbf{y}$$

If **V** is estimated, then the WLS estimator is not necessarily BLUE [29].

2.2.3 Seemingly Unrelated Regression and Multivariate Regression

Considering an experiment with *m* responses $y_1, y_2, \dots y_{\mathrm{m}}$ and *n* observations on each response, the set of linear equations for the i^{th} response in matrix notation is

$$\mathbf{y}_i = \mathbf{X}_i\boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i\,, \qquad i = 1,2,\dots,m$$

where $\mathbf{y}_i$ is the vector of observations on the i^{th} response, $\mathbf{X}_i$ is the design matrix, $\boldsymbol{\beta}_i$ is the vector of unknown parameters, $\boldsymbol{\varepsilon}_i$ is a random error vector associated with the i^{th} response. Each of these equations has the structure defined in (2.5).

The assumptions related to the error terms are as follows:

$$\mathrm{E}(\boldsymbol{\varepsilon}_i) = \mathbf{0} \;\; \forall i$$

$$\mathrm{Var}(\boldsymbol{\varepsilon}_i) = \sigma_{ii}\mathbf{I}_n \;\; \forall i$$

$$\mathrm{Cov}(\boldsymbol{\varepsilon}_i, \boldsymbol{\varepsilon}_k) = \sigma_{ik}\mathbf{I}_n \; \forall i,k \;\text{ where } i \neq k$$

In SUR formulation, these *m* models are stacked in one model

$$\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_m \end{bmatrix} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 & \mathbf{0} & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{X}_m \end{bmatrix} \begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_m \end{bmatrix} + \begin{bmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_m \end{bmatrix}$$

which can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Then, variance-covariance structure of $\boldsymbol{\varepsilon}$ can be expressed as

$$\mathrm{Cov}(\boldsymbol{\varepsilon}) = \mathrm{E}(\boldsymbol{\varepsilon}'\boldsymbol{\varepsilon}) = \mathbf{W} \otimes \mathbf{I}_n = \boldsymbol{\Omega}$$

where $\mathbf{W}$ is the $m \times m$ variance-covariance matrix of the responses and so do the error terms such that

$$\mathbf{W} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \cdot & \cdot & \sigma_{1m} \\ \sigma_{21} & \sigma_{22} & \cdot & \cdot & \sigma_{2m} \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \sigma_{m1} & \sigma_{m2} & \cdot & \cdot & \sigma_{mm} \end{bmatrix}$$

The operator $\otimes$ denotes the Kronecker product, then

$$\boldsymbol{\Omega} = \mathbf{W} \otimes \mathbf{I}_n = \begin{bmatrix} \sigma_{11}\mathbf{I}_n & \sigma_{12}\mathbf{I}_n & \cdot & \cdot & \sigma_{1m}\mathbf{I}_n \\ \sigma_{21}\mathbf{I}_n & \sigma_{22}\mathbf{I}_n & \cdot & \cdot & \sigma_{2m}\mathbf{I}_n \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \sigma_{m1}\mathbf{I}_n & \sigma_{m2}\mathbf{I}_n & \cdot & \cdot & \sigma_{mm}\mathbf{I}_n \end{bmatrix}$$

Accordingly, SUR allows that the error terms are correlated and the variances at each design setting are constant. Then, SUR estimator of $\boldsymbol{\beta}$ is obtained by applying the GLS method so that

$$\widehat{\boldsymbol{\beta}}_{\mathrm{SUR}} = (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{y}$$

Accordingly, the fitted values and the residuals are as given by the following equations:

$$\hat{\mathbf{y}}_{\mathbf{SUR}} = \mathbf{X}\,\widehat{\boldsymbol{\beta}}_{\mathbf{SUR}}$$

$$\hat{\boldsymbol{\varepsilon}}_{\mathbf{SUR}} = \mathbf{y} - \hat{\mathbf{y}}_{\mathbf{SUR}}$$

SUR estimator shows the following properties:

$$\mathbf{E}[\widehat{\boldsymbol{\beta}}_{\mathbf{SUR}}] = \mathbf{E}[(\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{y}] = \mathbf{E}[(\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}(\mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon})]$$
$$= \mathbf{E}[(\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\boldsymbol{\varepsilon}] = \boldsymbol{\beta}$$

$$\mathbf{Cov}(\widehat{\boldsymbol{\beta}}_{\mathbf{SUR}}) = \mathbf{Var}(\widehat{\boldsymbol{\beta}}_{\mathbf{SUR}}) = \mathbf{Var}[(\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{y}]$$
$$= (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{Var}(\mathbf{y})[(\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}]'$$
$$= (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\boldsymbol{\Omega}\,[(\boldsymbol{\Omega}')^{-1}\,X\;\;(\mathbf{X}'(\boldsymbol{\Omega}')^{-1}\,\mathbf{X})^{-1}]$$
$$= (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}(\mathbf{X}'(\boldsymbol{\Omega}')^{-1}\,X)(\mathbf{X}'(\boldsymbol{\Omega}')^{-1}\,\mathbf{X})^{-1} = (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1}$$

Also, assuming the error term is distributed multivariate normal

$$\widehat{\boldsymbol{\beta}}_{\mathrm{SUR}} \sim \mathrm{N}(\boldsymbol{\beta}, (\mathbf{X}'\boldsymbol{\Omega}^{-1}\,\mathbf{X})^{-1})$$

SUR is first introduced by Zellner [10]. Providing that **W** is known**,** SUR estimator is BLUE by Aitken's theorem [30]. However, if **W** is not known, then it needs to be estimated. In this case, SUR estimator may not be BLUE. There are many ways to estimate **W**. Estimating it by using the OLS residuals as Zellner [10] suggests is the most common way, that is

$$\widehat{\mathbf{W}} = \frac{\widehat{\boldsymbol{\varepsilon}}'_{\mathbf{OLS}}\,\widehat{\boldsymbol{\varepsilon}}_{\mathbf{OLS}}}{n} \tag{2.8}$$

Accordingly, MVR and SUR fit these models to the data simultaneously and by taking the correlation among responses into consideration. MVR is a special case of SUR in which the responses are modeled by the same set of predictors. Thus, in MVR, there is a possibility that some of the models include insignificant terms. Since MVR is a special case of SUR, we only present the formulation of SUR here. However, there is an alternative way to formulate MVR. For this formulation and more details on MVR, multivariate analysis literature such as Johnson and Wichern [31], Mukhopadhyay [32] and Haase [33] can be referred to.

For more details on SUR, [30] can be referred to.

2.3 Performance Measures Used to Compare the Regression Methods

In our study, we are interested to examine and compare the accuracy and precision of the estimation methods presented in the previous section. To evaluate performances of the methods we have used the following performance measures. The corresponding formulations are written considering the response model in (2.4).

- Coefficient of Determination, R^2: It reveals the amount of the variation in response due to the model. A high value of this quantity indicates that the model fits the data well.

$$R^2 = 1 - \frac{\text{SSE}}{\text{SST}} = 1 - \frac{\sum_{j=1}^{n}\left(y_{(j)} - \hat{y}_{(j)}\right)^2}{\sum_{j=1}^{n}\left(y_{(j)} - \bar{y}\right)^2}$$

$$\text{where } \bar{y} = \frac{1}{n}\sum_{j=1}^{n} y_{(j)}$$

One disadvantage of using R^2 is that it does not take the number of estimated parameters (complexity of the model) into account, which causes R^2 to increase each time a parameter is added to the model. In other words, the highest R^2 does not necessarily mean that the corresponding model is the best.

- Mean Square Error (MSE): It is a measure which considers both the number of estimated parameters in the model and the residual sum of squares. A small MSE value is desired to ensure a better model.

$$\text{MSE} = \frac{\text{SSE}}{n - (number\ of\ estimated\ \beta\ parameters)} = \frac{\sum_{i=1}^{n}\left(y_{(j)} - \hat{y}_{(j)}\right)^2}{n - p}$$

The definition of R^2 and MSE can easily be found in any statistics text book such as Mendenhall and Sincich [34], Kutner et al. [35], Montgomery et al. [5].

Note that when WLS is applied, softwares like Minitab and R calculate SSE and SST by considering the weights as follows:

$$\text{weighted SSE} = \sum_{j=1}^{n} w_j \left(y_{(j)} - \hat{y}_{(j)}\right)^2$$

$$\text{weighted SST} = \sum_{i=1}^{n} w_j \left(y_{(j)} - \bar{y}\right)^2$$

- Prediction Variance of Unknown Model Parameters: All estimation methods considered in the scope of this study and defined in the previous section produce unbiased estimators for the unknown model parameters. However, their efficiency, i.e. variance of the estimators, varies in different circumstances. For this reason, we examine the variance-covariance matrix of the estimated model parameters. In order to evaluate this matrix with a single numerical value, we use its trace and determinant which are regarded as overall measures of dispersion.

  Let $\widehat{\boldsymbol{\beta}}$ be the estimator of $\boldsymbol{\beta}$. Then, we report $\text{trace}[\mathbf{Cov}(\widehat{\boldsymbol{\beta}})]$ and $\det[\mathbf{Cov}(\widehat{\boldsymbol{\beta}})]$. Trace of the matrix gives the sum of variances of the estimated model parameters. It is also called as total variation. However, this measure does not take the correlation among the parameters into consideration. Thus, we also examine the determinant of the matrix which is also called generalized variance. The determinant being large denotes the data are dispersed much.

- Variance of the Predicted Mean Response: For some selected points from the experiment design, we examine the prediction variance. We have chosen two points: A center point and a corner point of a central composite design, typically used in developing response surface models. Let $\mathbf{x_0}$ be the column vector of predictors at such a chosen point and $\widehat{\boldsymbol{\beta}}$ be the estimator of $\boldsymbol{\beta}$. Then, predicted mean response is

  $$\widehat{\mathrm{E}}\,(\mathbf{y}) = \mathbf{x}_0'\widehat{\boldsymbol{\beta}}$$

  and the prediction variance of the estimated mean response at $\mathbf{x_0}$ is

  $$\mathrm{Var}(\widehat{\mathrm{E}}\,(\mathbf{y})) = \mathrm{Var}\,(\mathbf{x_0}\widehat{\boldsymbol{\beta}}) = \mathbf{x}_0'\,\mathrm{Var}(\widehat{\boldsymbol{\beta}})\,\mathbf{x_0}$$

For more details on the measures defined above, Johnson and Wichern [31] can be referred to.

- Hellinger Distance: Hellinger distance is one of the statistical distance metrics used to measure divergence between any two probability distributions.

  Pardo [36], and Abou-Moustafa and Ferrie [37] give the derivation of Hellinger distance for two multivariate normal distributions. Let P and Q be two multivariate normal distribution such that $\mathrm{P} \sim \mathrm{N}(\boldsymbol{\mu_1}, \boldsymbol{\Sigma_1})$ and $\mathrm{Q} \sim \mathrm{N}(\boldsymbol{\mu_2}, \boldsymbol{\Sigma_2})$. Then, Hellinger distance for such two multivariate normal distributionsas follows:

$$d_{\mathrm{H}} = \sqrt{2\left(1 - \frac{\det(\boldsymbol{\Sigma_1})^{\frac{1}{4}} \det(\boldsymbol{\Sigma_2})^{\frac{1}{4}}}{\det\left(\frac{\boldsymbol{\Sigma_1}+\boldsymbol{\Sigma_2}}{2}\right)^{\frac{1}{2}}} \exp\left(-\frac{1}{8}\left(\boldsymbol{\mu_1}-\boldsymbol{\mu_2}\right)'\left(\frac{\boldsymbol{\Sigma_1}+\boldsymbol{\Sigma_2}}{2}\right)^{-1}\left(\boldsymbol{\mu_1}-\boldsymbol{\mu_2}\right)\right)\right)}$$

By definition, $0 \leq d_{\mathrm{H}} \leq 1$. We use it to measure the distance between true and predicted distributions of a single observation defined at a certain design point. It also gives an idea about which prediction region is closer to the true region.

2.4 Joint Confidence and Prediction Regions by Bootstrap Technique

Ouyang et al. [25] define two categories for the approaches dealing with the model uncertainty in a MRDPO problem. First category includes the approaches based on ensemble of models obtained using different methods, like Zhou et al. [38] do, while the approaches in the second category are based on providing confidence intervals of estimated values and using this information in the optimization process. Considering the approaches in the latter category, we provide joint confidence and prediction regions for the multiple mean responses by using the bootstrap technique.

We provide joint regions instead of simultaneous confidence intervals because it is more precise. If we construct separate confidence intervals by specifying some coverage probability, we cannot obtain the same probability by taking all these intervals together. That is, to enable the specified coverage probability overall, we need to construct simultaneous intervals at larger probability levels [31].

Bootstrap technique was first introduced by Efron [39]. It is commonly used to evaluate the accuracy of the estimators, no matter how the statistic estimated is complicated. It is a computer-intensive method, but simple to apply. The idea of the method is to generate bootstrap samples from the original data (by resampling with replacement) and to calculate the statistic of interest for each of these samples. In this way, information about the empirical distribution of the statistic is obtained. Let Q be the statistic of interest. Then, the general idea of bootstrap can be represented as in Figure 2.2. For more details on bootstrap methods and their application, Tibshirani and Efron [40], [41], Diciccio and Efron [42] and can be referred to.

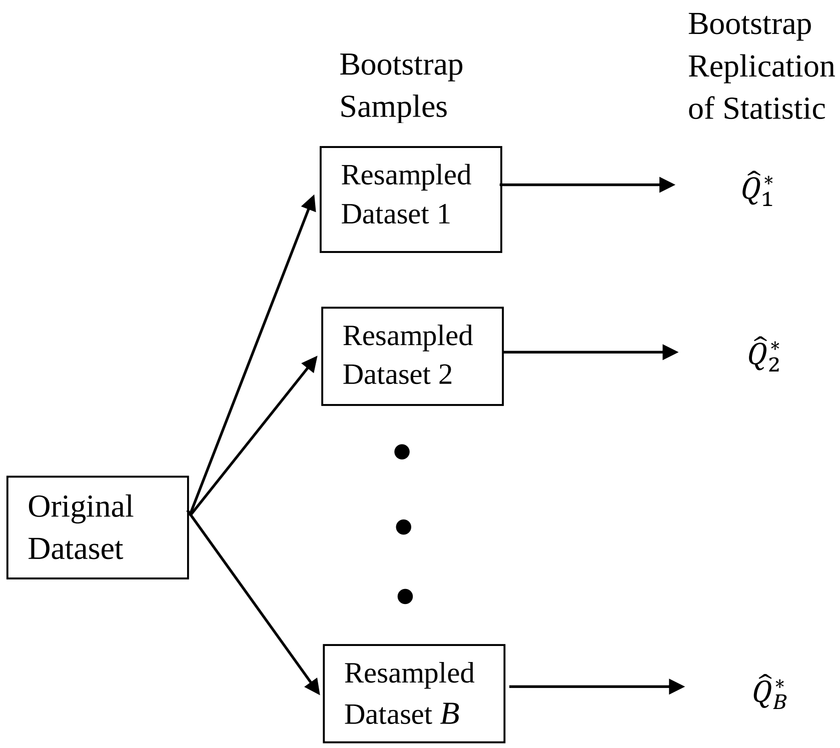

Figure 2.2 A representation of the idea in bootstrapping (resampling)

In our study, we apply bootstrap technique for several reasons. First, it is simple to apply as stated before. Second, to the best of our knowledge, there are no theoretical expressions defined for the confidence and prediction regions in the context of SUR (except when it is equivalent to MVR). Besides, obtaining such expressions are not straightforward. Also, we compare the theoretical confidence and prediction regions with the regions obtained by bootstrap for MVR. The regions are satisfactorily close to each other, so we conclude that bootstrap regions work well.

Park [43] and Davison and Hinkley [44] present two ways of using the bootstrap samples to obtain joint confidence regions when multiple parameters are estimated. One way is to construct a rectangular region based on the Bonferroni approach. The other way is to construct an elliptical region by assuming multivariate normal distribution. By adopting the second way, we follow the procedure given in Park [43] and Davison and Hinkley [44].

Let $\boldsymbol{\theta}$ be the vector of unknown parameters and $\widehat{\boldsymbol{\theta}}$ be an unbiased estimator of it. Then, a generalized squared distance can be expressed by

$$Q = \left(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right)' (\boldsymbol{\Sigma}_{\widehat{\boldsymbol{\theta}}})^{-\mathbf{1}} \left(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right)$$

where $\boldsymbol{\Sigma}_{\widehat{\boldsymbol{\theta}}}$ is the variance-covariance matrix of $\widehat{\boldsymbol{\theta}}$. Generating B bootstrap samples and calculating Q for each of these samples, 100 (1-α)% confidence region for $\boldsymbol{\theta}$ can be obtained by

$$\left(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right)' (\boldsymbol{\Sigma}_{\widehat{\boldsymbol{\theta}}})^{-\mathbf{1}} \left(\widehat{\boldsymbol{\theta}} - \boldsymbol{\theta}\right) \leq q^*_{[(1+\mathrm{B})(1-\alpha)]}$$

where $q^*_{[i]}$ represents the i$^{\text{th}}$ highest value in the sorted bootstrap estimates of Q. The superscript notation is used to indicate that it was a bootstrap value.

To calculate bootstrap estimates of Q, we need to use an estimator of $\boldsymbol{\Sigma}_{\widehat{\boldsymbol{\theta}}}$. One way to find such an estimator, let say $\widehat{\boldsymbol{\Sigma}}^*_{\widehat{\boldsymbol{\theta}}}$, is as follows:

$$\widehat{\boldsymbol{\Sigma}}^{*}_{\widehat{\boldsymbol{\theta}}} = \frac{1}{1 - I} \sum_{i=1}^{I} \left(\widehat{\boldsymbol{\theta}}^{**}_{i} - \overline{\boldsymbol{\theta}}^{**}\right)\left(\widehat{\boldsymbol{\theta}}^{**}_{i} - \overline{\boldsymbol{\theta}}^{**}\right)'$$

$$\text{where } \overline{\boldsymbol{\theta}}^{**} = \frac{1}{I}\sum_{\mathrm{i}=1}^{I} \widehat{\boldsymbol{\theta}}^{**}_{i}$$

and $\widehat{\boldsymbol{\theta}}^{**}_{1}, \widehat{\boldsymbol{\theta}}^{**}_{2}, \ldots, \widehat{\boldsymbol{\theta}}^{**}_{I}$ are resampled among B bootstrap estimates of $\boldsymbol{\theta}$.

Here, I is typically a value taken between 50 and 200.

CHAPTER 3

DEVELOPMENT OF REGRESSION MODELS, EXPERIMENTS, DATA, CONFIDENCE AND PREDICTION REGIONS FOR COMPARISON

In this chapter, we present our comparison approach. We first explain how we apply the regression methods simultaneously to model each mean response. Then, we design the experiments (scenarios) and generate data accordingly to evaluate and compare estimation and prediction errors of the methods. While designing the scenarios, we are particularly interested in answering the following research question: Under which circumstances (violation of certain assumptions, being at a far point from the design center, number of replications etc.), estimation errors associated with model parameters and prediction errors associated with individual observations are high in MRDPO problems?

Furthermore, we provide a detailed explanation about how we develop the confidence and prediction regions using the bootstrap technique.

3.1 Simultaneous Modeling of the Mean Responses

We can express all linear regression methods under consideration with the same formulation of SUR. Let $y_1, y_2, \ldots y_m$ be the responses to be estimated. Assuming there are *n* observations at each design point for each response and *d* is the number of design points in the data collection experiment, the model for the i^{th} response in matrix notation is

$$\mathbf{y}_i = \mathbf{X}_i \boldsymbol{\beta}_i + \boldsymbol{\varepsilon}_i \,, \qquad i = 1,2, \ldots, m$$

where $\mathbf{y}_i$ is the vector of observations, $\mathbf{X}_i$ the design matrix, $\boldsymbol{\beta}_i$ is the vector of unknown parameters, $\boldsymbol{\varepsilon}_i$ is a random error vector, which are all associated with the i^{th} response.

These *m* models can be stacked in one model as follows:

$$\begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_m \end{bmatrix}_{mnd\times 1} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{0} & \mathbf{0} & \dots & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_2 & \mathbf{0} & \dots & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots & \mathbf{X}_m \end{bmatrix}_{mnd\times k} \begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_m \end{bmatrix}_{k\times 1} + \begin{bmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_m \end{bmatrix}_{mnd\times 1}$$

which can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Note that *k* represents the total number of estimated parameters for all responses. For example, if all design matrices, $\mathbf{X}_1$, $\mathbf{X}_2$, …, $\mathbf{X}_m$, have the same set of predictors as given in (2.5), *k* equals to $\left(1 + 2r + \binom{r}{2}\right) m$.

Let the variance-covariance structure of $\boldsymbol{\varepsilon}$ be defined as follows:

$$\mathrm{Cov}(\boldsymbol{\varepsilon}) = \boldsymbol{\Sigma} \otimes \mathbf{I}_n$$

where

$$\boldsymbol{\Sigma} = \begin{bmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\Sigma}_{12} & \dots & \boldsymbol{\Sigma}_{1m} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_{22} & \dots & \boldsymbol{\Sigma}_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{\Sigma}_{m1} & \boldsymbol{\Sigma}_{m2} & \dots & \boldsymbol{\Sigma}_{mm} \end{bmatrix}_{md\times md}$$

such that

$$\boldsymbol{\Sigma}_{ij} = \boldsymbol{\Sigma}_{ji} = \begin{bmatrix} \sigma_{ij1} & 0 & \dots & 0 \\ 0 & \sigma_{ij2} & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_{ijd} \end{bmatrix}_{d\times d} \quad \text{where } i, j = 1, 2, \dots, m$$

Then, the estimator of $\boldsymbol{\beta}$ is defined as

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}'(\boldsymbol{\Sigma} \otimes \mathbf{I}_n)^{-1}\,\mathbf{X})^{-1}\mathbf{X}'(\boldsymbol{\Sigma} \otimes \mathbf{I}_n)^{-1}\,\mathbf{y}$$

Depending on $\boldsymbol{\Sigma}$, the estimator is named.

Table 3.1 Summary of variance-covariance structures of the regression methods

Method	$\boldsymbol{\Sigma}_{ii}$	$\boldsymbol{\Sigma}_{ij}\ (i \neq j)$
OLS	$\boldsymbol{\Sigma}_{ii} = \sigma_{ii}\mathbf{I}_d \quad \forall i$	$\boldsymbol{\Sigma}_{ij} = \mathbf{0} \quad \forall i, j$
GLS (WLS)	$\boldsymbol{\Sigma}_{ii} = \sigma_{ii}\mathbf{V}_d \quad \forall i$, $\mathbf{V}_d$ is diagonal matrix, $(\mathbf{V}_d \neq \mathrm{I}_d)$	$\boldsymbol{\Sigma}_{ij} = \mathbf{0} \quad \forall i, j$
SUR (MVR)	$\boldsymbol{\Sigma}_{ii} = \sigma_{ii}\mathbf{I}_d \quad \forall i$	$\boldsymbol{\Sigma}_{ij} = \sigma_{ij}\mathbf{I}_d \quad \forall i, j$

The estimator shows the following properties:

$$\mathbf{E}[\widehat{\boldsymbol{\beta}}] = \boldsymbol{\beta}$$

$$\mathbf{Cov}(\widehat{\boldsymbol{\beta}}) = \mathbf{Var}(\widehat{\boldsymbol{\beta}}) = (\mathbf{X}'(\boldsymbol{\Sigma} \otimes \mathbf{I_n})^{-\mathbf{1}}\,\mathbf{X})^{-\mathbf{1}}$$

3.2 Design of Comparison Experiments

In our comparison study, we consider an MRPDO problem in a chemical process presented by Ko et al. [7]. In this problem, there are two responses of interest: the conversion of a polymer (y_1) and its thermal activity (y_2). Also, there are three controllable factors affecting the responses which are reaction time (x_1), reaction temperature (x_2), and the amount of catalyst (x_3). The aim of the problem is to determine the best levels of the controllable factors so as to maximize y_1 and make y_2 as close as possible to a target value of 57.5. The acceptable ranges for y_1 and y_2 are defined as (80,100) and (55,60), respectively.

We do not directly use the experimental results presented by Ko et al. [7]. We only use the design of experiments, i. e. design settings for the controllable factors, which is given in Table 3.2. We later define some true relationships between the responses and the controllable factors. In defining those relationships, we choose model parameters close to those of the models reported by Ko et al. [7], to have a meaningful MRDPO problem.

Table 3.2 Results of the polymer experiment

Design Setting	x_1	x_2	x_3
1	-1	-1	-1
2	1	-1	-1
3	-1	1	-1
4	1	1	-1
5	-1	-1	1
6	1	-1	1
7	-1	1	1
8	1	1	1
9	-1.68	0	0
10	1.68	0	0
11	0	-1.68	0
12	0	1.68	0
13	0	0	-1.68
14	0	0	1.68
15	0	0	0
16	0	0	0
17	0	0	0
18	0	0	0
19	0	0	0
20	0	0	0

In order to generate our comparison cases or scenarios, we first assume true functional relationships between the responses and the controllable factors. Also, we make some assumptions related to the error terms in these functions. Then, at each design setting in Table 3.2, we generate some replications by simulation using the presumed true models and error distributions. Then, we apply the regression methods separately to the generated data to obtain second-order surface models for the mean responses.

We analyze twelve scenarios defined in Table 3.3 to compare the regression methods for this example problem. These scenarios are systematically generated by statistical design of experiments. The experiment considers the following factors: number of replications, error variance homogeneity and correlation between the responses. Number of replications assumes two levels: 5 and 25. Error variance is taken as either homogeneous or heterogeneous. Finally, three correlation levels for the responses are studied: 0, 0.3 and 0.9 as shown in Table 3.3 to see the effects of changing levels of these factors on performances of the methods. The first eight scenarios constitute a fraction of the full factorial design of the comparison experiments, which has twelve scenarios in total. The remaining four scenarios have not been studied, since no appropriate linear regression method is readily available in the literature, to the best of our knowledge, to use in these scenarios. In the first eight scenarios, for simplicity, the same set of predictors are used in modeling the responses using all regression methods. For all scenarios, data are collected by simulation based on the true models and error distributions, and the performance measures are computed at two different design points: center and corner of the central composite design shown in Table 3.2.

Effect of using a different set of predictors for a different response can be observed better when a regression method, such as SUR, allows use of a different set of predictors while the others do not. Therefore, four additional scenarios shown in the last four rows of Table 3.3. are considered to study the effect of having a different set of predictors for modeling a response.

In Table 3.3, it is shown which method is the most appropriate or applicable for each scenario based on their assumptions. It is seen that for some scenarios, some of the methods are equivalent.

When the sets of predictors of the responses are all the same, we assume the true functional relationship between the responses and the controllable factors are as follows:

$$y_1 = \mathrm{f}_1(x) + \varepsilon_1 \text{ where}$$

$$\mathrm{f}_1(x) = 80 + x_1 + 4x_2 + 6x_3 - 2x_1^2 + 3x_2^2 - 5x_3^2 + 2x_1x_2 + 12x_1x_3 - 4x_2x_3$$

$$y_2 = \mathrm{f}_2(x) + \varepsilon_2 \text{ where}$$

$$\mathrm{f}_2(x) = 60 + 4x_1 + x_2 + 3x_3 + x_1^2 + x_2^2 - x_3^2 - x_1x_2 - x_1x_3 + x_2x_3 \qquad (3.1)$$

Table 3.3 Scenarios considered in the comparison study (A: applicable, NA: not applicable)

Scenario #	Number of replications, n	Heteroscedasticity	Correlation coefficient, ρ	Position of the point	Set of predictors of the responses	OLS	WLS	MVR	SUR
1	5	No	0	center/corner	Same	A	NA	equal to OLS	equal to MVR
2	25	No	0	center/corner	Same	A	NA	equal to OLS	equal to MVR
3	5	Yes	0	center/corner	Same	NA	A	NA	equal to MVR
4	25	Yes	0	center/corner	Same	NA	A	NA	equal to MVR
5	5	No	0.3	center/corner	Same	NA	NA	A	equal to MVR
6	25	No	0.3	center/corner	Same	NA	NA	A	equal to MVR
7	5	No	0.9	center/corner	Same	NA	NA	A	equal to MVR
8	25	No	0.9	center/corner	Same	NA	NA	A	equal to MVR
9	5	No	0.3	center/corner	Different	NA	NA	NA	A
10	25	No	0.3	center/corner	Different	NA	NA	NA	A
11	5	No	0.9	center/corner	Different	NA	NA	NA	A
12	25	No	0.9	center/corner	Different	NA	NA	NA	A

Accordingly, while fitting the second-order surface models, we consider all terms are significant for both responses. In such a case, SUR is equivalent to MVR.

When the sets of predictors of the responses are taken different, we consider another true functional relationship between the second response and controllable variables, that is, instead of the equation (3.1), we assume the following equation

$$\mathrm{f}_2(x) = 60 + 4x_1 + 3x_3$$

In this case, we expect different significant terms for each response, so SUR is different than MVR, and it dominates MVR because for some responses MVR includes insignificant terms in the model.

In the true functions defined above, ε_1 and ε_2 are called as the random error terms. Let $\mu_{\mathbf{0}}$ be the mean vector and $\mathbf{\Sigma_0}(\mathbf{x})$ be the variance-covariance matrix of the error terms. We assume that error terms are distributed as

$$\boldsymbol{\varepsilon} = \begin{bmatrix} \boldsymbol{\varepsilon_1} \\ \boldsymbol{\varepsilon_2} \end{bmatrix} \sim \mathrm{N}(\mu_{\mathbf{0}}, \mathbf{\Sigma_0}(\mathbf{x}))$$

$$\text{where } \mu_{\mathbf{0}} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \qquad \mathbf{\Sigma_0}(\mathbf{x}) = \begin{bmatrix} \sigma_{11}(\mathbf{x}) & \sigma_{12}(\mathbf{x}) \\ \sigma_{21}(\mathbf{x}) & \sigma_{22}(\mathbf{x}) \end{bmatrix} \text{ and } \mathbf{x} = (x_1,\ x_2,\ x_3)$$

$\sigma_{11}(\mathbf{x})$ and $\sigma_{22}(\mathbf{x})$ are the variances of $\boldsymbol{\varepsilon_1}$ and $\boldsymbol{\varepsilon_2}$ at setting $\mathbf{x}$ while $\sigma_{12}(\mathbf{x})$ and $\sigma_{21}(\mathbf{x})$ are covariances between these two terms at setting $\mathbf{x}$ such that

$$\sigma_{12}(\mathbf{x}) = \sigma_{21}(\mathbf{x}) = \rho\sqrt{\sigma_{11}(\mathbf{x})\sigma_{22}(\mathbf{x})}$$

where ρ is the Pearson correlation coefficient.

When there is no heteroscedasticity, the following functions are presumed for the variances.

$$\sigma_{11}(\mathbf{x}) = e^3 \text{ and } \sigma_{22}(\mathbf{x}) = e^2$$

In the existence of heteroscedasticity, true functions of the variances are taken as

$$\sigma_{11}(\mathbf{x}) = e^{3-x_1^2-3x_3^2} \text{ and } \sigma_{22}(\mathbf{x}) = e^{2-2x_1^2-x_3^2} \tag{3.2}$$

The assumed functions for the variances in (3.2) are obtained from Ko et al. [7].

We generate data according to the number of replications (n=5 or n=25) and try to observe the effect of number of replications in the quality of estimation and predictions. Also, for the cases in which correlation among the error terms exists, we take into account the correlation level in generating the data (ρ=0 or 0.3 or 0.9) to draw conclusions about the behavior of the methods while correlation increases. Additionally, for some selected points from the experiment design, we examine the prediction variance. We have chosen two points of the design: The center point where all controllable factors are set to zero and a corner point where all controllable factors are set to one.

While applying methods except OLS, we need to use the variance-covariance matrix of the responses, which is most probably unknown. Still, we leave the variance and correlation estimation out of our scope. We simply use sample variances while applying WLS. In this manner, number of replications affects the estimation of variance-covariance matrix, as well. In order to apply SUR, we estimate the variance-covariance matrix based on the OLS residuals as Zellner [10] suggests. Still, to exclude effect of the accuracy in the estimation of variance-covariance matrix on the performances of the methods, we also make analyses under the assumption that variance-covariance matrix of the mean responses is known.

Once we generate data under a scenario, we test it to ensure that it satisfies the assumptions of that scenario. First, we test for heteroscedasticity. There are plenty of formal tests such as Park test, Glejser's test, Spearman's rank correlation test, Goldfeld-Quandt test, Bartlett's test, Breusch-Pagan test and White's test [29]. These are commonly referenced in econometrics literature and most of them are based on the examination of the OLS residuals. However, in statistics literature, we mostly encounter with Bartlett's and Levene's tests which are utilized to test equal variances across samples. If the data tested is normally distributed, Bartlett test can be used. However, if not, Levene's test is a better alternative since it is less sensitive to the distribution of the data. We apply Levene's test for heteroscedasticity. We also test whether there is a correlation among the responses at a defined design setting or not. All generated data meet the scenario requirements according to these tests.

3.3 Application of Bootstrap Technique to Obtain Joint Confidence and Prediction Regions

We construct elliptical confidence and prediction regions following the procedure described in Section 2.4. First, we set B=999 and α=0.10 and define $\boldsymbol{\theta}$ as $\mathbf{y}$. Then, we follow these steps:

1) Generating bootstrap samples (resampling): At each design point, we sample from the original data with replacement and with a number of replications n as seen in Table 3.4. We call the resulting new experimental data a bootstrap sample. In this manner, we produce B bootstrap samples.

Table 3.4 A Representation of resampling in this study

Design Point	Observation Number	x_1	x_2	x_3	y_1	y_2		y_1^*	y_2^*
1	1	-1	-1	-1	74.74	52.52	sampling with replacement, sample size n	74.74	52.52
	2	-1	-1	-1	73.99	52.76		74.74	52.52
	⋮	⋮	⋮	⋮	⋮	⋮	$\longrightarrow$	⋮	⋮
	n	-1	-1	-1	74.58	51.03		75.58	51.03
2	1	1	-1	-1	48.39	63.86		49.31	64.19
	2	1	-1	-1	49.37	64.07	sampling with replacement, sample size n	48.11	63.84
	⋮	⋮	⋮	⋮	⋮	⋮		⋮	⋮
	n	1	-1	-1	48.11	63.84	$\longrightarrow$	48.11	63.84
⋮	⋮	⋮	⋮	⋮	⋮	⋮		⋮	⋮

2) Applying the regression method: For each bootstrap sample, we apply the regression method and make prediction at the point of interest (either the center or the corner point), $\hat{\mathbf{y}}_{\mathrm{b}}^{*} = \begin{bmatrix} \hat{y}_{1,b}^{*} \\ \hat{y}_{2,b}^{*} \end{bmatrix}$.

3) Obtaining bootstrap estimate of variance-covariance matrix of $\hat{\mathbf{y}}$, $\widehat{\mathbf{\Sigma}}_{\hat{\mathbf{y}}}^{*}$: $\hat{\mathbf{y}}_{1}^{**}, \hat{\mathbf{y}}_{2}^{**}, \dots, \hat{\mathbf{y}}_{I}^{**}$ are resampled among B bootstrap estimates of **y,** and $\widehat{\mathbf{\Sigma}}_{\hat{\mathbf{y}}}^{*}$ calculated by

$$\widehat{\mathbf{\Sigma}}_{\hat{\mathbf{y}}}^{*} = \frac{1}{1-I} \sum_{i=1}^{I} (\hat{\mathbf{y}}_{i}^{**} - \bar{\mathbf{y}}^{**})(\hat{\mathbf{y}}_{i}^{**} - \bar{\mathbf{y}}^{**})'$$

where $\bar{\mathbf{y}}^{**} = \frac{1}{I} \sum_{i=1}^{I} \hat{\mathbf{y}}_{i}^{**}$ and I=150.

4) Calculating bootstrap estimates of the statistic of interest, Q: Q is the generalized squared distance and its bootstrap estimates are calculated by

$$\hat{q}_{b}^{*} = (\hat{\mathbf{y}}_{\mathrm{b}}^{*} - \hat{\mathbf{y}})' \left(\widehat{\mathbf{\Sigma}}_{\hat{\mathbf{y}}}^{*}\right)^{-\mathbf{1}} (\hat{\mathbf{y}}_{\mathrm{b}}^{*} - \hat{\mathbf{y}})$$

5) Constructing confidence region for $E(\mathbf{y})$: 90% elliptical confidence region for **y** is constructed by

$$(\hat{\mathbf{y}} - \mathbf{y})' \left(\mathbf{\Sigma}_{\hat{\mathbf{y}}}\right)^{-\mathbf{1}} (\hat{\mathbf{y}} - \mathbf{y}) \leq q_{[\mathbf{900}]}^{*}$$

$q_{[\mathbf{900}]}^{*}$ is the 900$^{\text{th}}$ highest value in the sorted bootstrap estimates of Q.

To obtain the prediction region, we need to consider the inherent variation in **y,** as well [25]. Suppose it is has a variance-covariance matrix defined by $\mathbf{\Sigma}_{\mathbf{y}}$. Then, by making analogy to the theoretical prediction ellipsoid of MVR given by Johnson and Wichern [31], we suggest to construct 90% prediction region for **y** by

$$(\hat{\mathbf{y}} - \mathbf{y})' \left(\mathbf{\Sigma}_{\mathbf{y}} + \mathbf{\Sigma}_{\hat{\mathbf{y}}}\right)^{-\mathbf{1}} (\hat{\mathbf{y}} - \mathbf{y}) \leq q_{[\mathbf{900}]}^{*}$$

$\mathbf{\Sigma}_{\mathbf{y}}$ is generally unknown and needs to be estimated. We use MSE values to estimate its elements, i.e. variances, while applying OLS and WLS. However, for MVR and SUR, we estimate it based on the OLS residuals as given in (2.8).

CHAPTER 4

NUMERICAL RESULTS AND DISCUSSION

In this chapter, we show the computational results for each scenario defined in the previous chapter and give some discussions indicating how the methods applied perform in each situation. Besides, we provide joint confidence and prediction regions for the estimated mean responses at the center and corner points of the experimental design by using the bootstrap technique.

Note that results presented in the following sections include weighted performance measures in parenthesis when WLS is applied.

4.1 Scenarios 1-2: OLS Case

OLS is applicable when the responses are not correlated and the error variances are homogeneous. True mean, variance and covariance values at each design point of the experimental design for this case, which are all predetermined, are given in Table A.1 in Appendix A. Data in scenarios 1 and 2 are generated accordingly. OLS is applicable for both of the scenarios. The only difference between these scenarios is the number of replications. We make an analysis by choosing different numbers of replications (n=5 and n=25) and try to observe the effect of number of replications on quality of the predictions. Generated data are given in Table A.2 for scenario 1 and in Table A.3 for scenario 2. After the data are generated, second-order response surface models are fitted to the responses by applying all regression methods under consideration, and performances of them are analyzed. Estimated model coefficients and predictions made at the center and the corner points of the designed experiment are given in Table A.4 through Table A.9.

Table 4.1 Performance measures (scenario 1)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
trace[Cov($\hat{\boldsymbol{\beta}}$)]	5.332	4.685	3.877	4.216
det[Cov($\hat{\boldsymbol{\beta}}$)]	872.241 x10^{-17}	24.325 x10^{-17}	0.097 x10^{-17}	1.525 x10^{-17}
MSE_1	18.548	18.548	18.924 (1.182)	18.548
MSE_2	5.594	5.594	5.644 (0.962)	5.594
R_1^2	0.883	0.883	0.881 (0.885)	0.883
R_2^2	0.816	0.816	0.814 (0.882)	0.816

Table 4.2 Performance measures at the center point (scenario 1)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.668	0.617	0.285	0.555
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.246	0.186	0.176	0.167
d_{H}	0.159	0.196	0.936	0.264

Table 4.3 Performance measures at the corner point (scenario 1)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	2.692	2.486	1.605	2.237
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.990	0.750	0.556	0.675
d_{H}	0.242	0.272	0.863	0.319

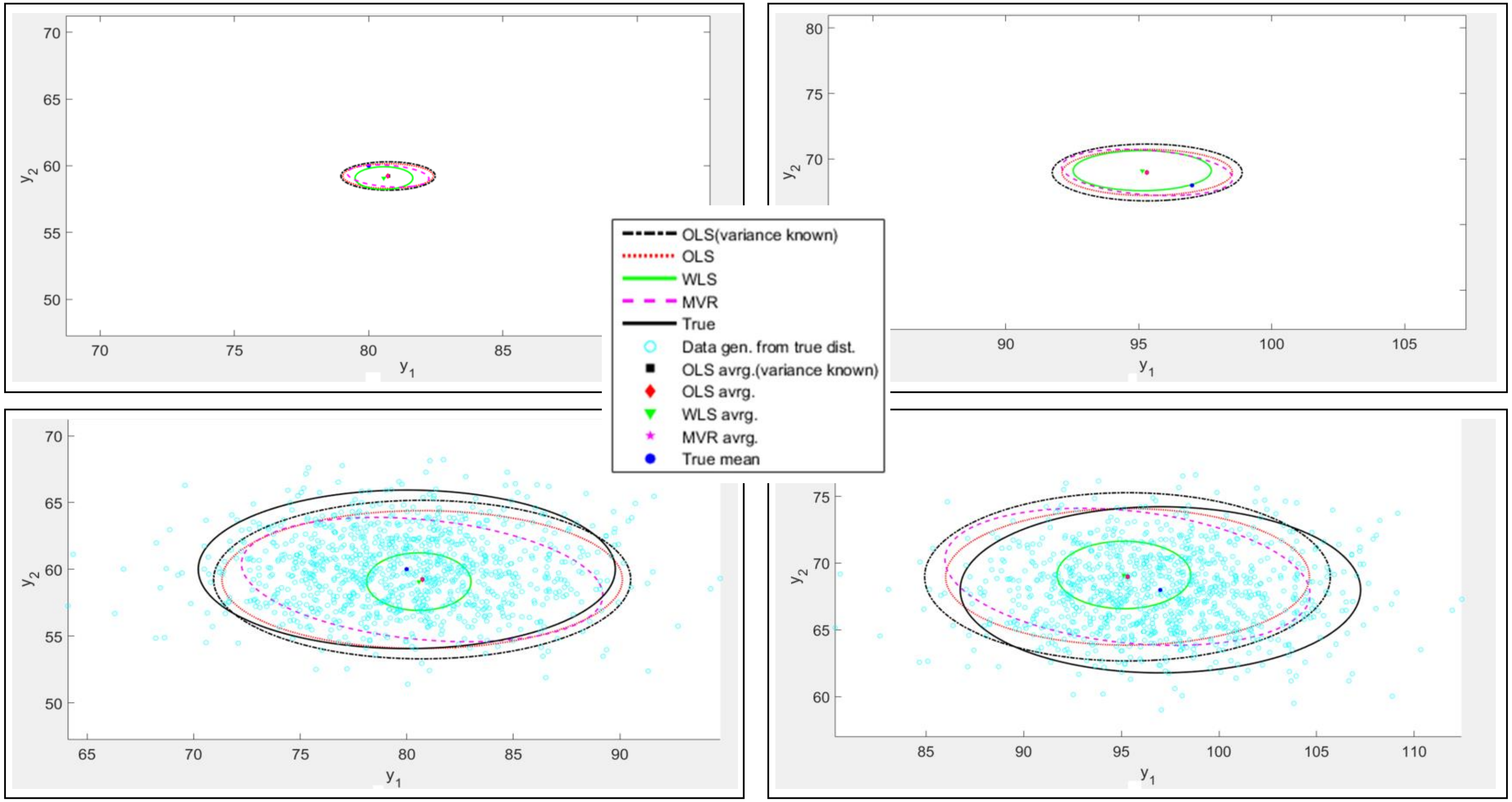

Figure 4.1 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 1)

Table 4.4 Performance measures (scenario 2)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
trace[Cov($\widehat{\boldsymbol{\beta}}$)]	1.066	0.951	0.927	0.932
det[Cov($\widehat{\boldsymbol{\beta}}$)]	91.461x10^{-30}	7.301 x10^{-30}	2.706 x10^{-30}	4.851 x10^{-30}
MSE_1	18.167	18.167	18.176 (1.004)	18.167
MSE_2	6.345	6.345	6.346 (1.004)	6.345
R_1^2	0.871	0.871	0.871 (0.881)	0.871
R_2^2	0.776	0.776	0.776 (0.782)	0.776

Table 4.5 Performance measures at the center point (scenario 2)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.134	0.121	0.126	0.118
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.049	0.042	0.039	0.041
d_{H}	0.063	0.091	0.959	0.099

Table 4.6 Performance measures at the corner point (scenario 2)

Performance Measures	OLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.538	0.487	0.555	0.477
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.198	0.170	0.193	0.167
d_{H}	0.058	0.088	0.906	0.096

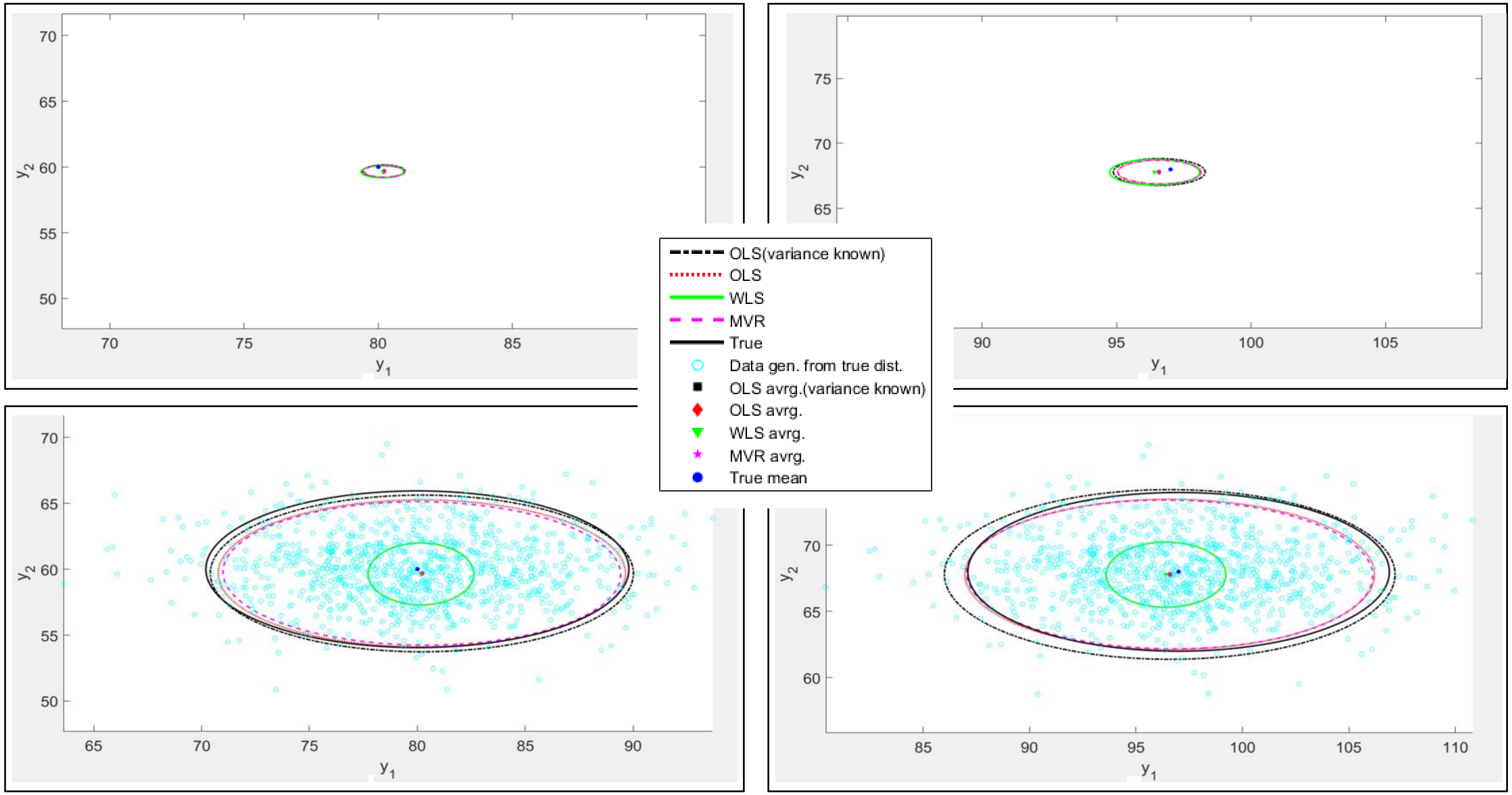

Figure 4.2 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 2)

Scenarios 1 and 2 have the circumstances that OLS is appropriate for use. Furthermore, OLS is known as BLUE if the variance-covariance matrix of the error terms is known. Still, for this particular example, we observe that both WLS and MVR seem to outperform in terms of the dispersion of the estimated parameters, i.e. they estimate $\boldsymbol{\beta}$ with lower values of trace[Cov($\widehat{\boldsymbol{\beta}}$)] and det[Cov($\widehat{\boldsymbol{\beta}}$)]. Accordingly, they predict mean responses $\widehat{\mathrm{E}}(y_1)$ and $\widehat{\mathrm{E}}(y_2)$ with smaller variances at the center and corner points of the experimental design. However, these methods use estimated variance-covariance matrix of the responses: Sample variances are used while applying WLS and an estimation is made based on OLS residuals to apply MVR. Moreover, when the variance-covariance matrix is assumed to be unknown, OLS underestimates the variances too (MSE values are used as the variance estimates of the responses in this case). Thus, it is seen that these measures are affected by the accuracy in estimation of the variance-covariance matrix. When the number of replications is increased in scenario 2, variance-covariance matrices used are estimated more accurately as well. Hence, values of trace[Cov($\widehat{\boldsymbol{\beta}}$)] and det[Cov($\widehat{\boldsymbol{\beta}}$)] decrease and performances of the methods get closer to the OLS estimation with known variance-covariance matrix.

Considering MSE and R^2, WLS seems to be slightly worse. However, if the measures of WLS given in parenthesis are considered, which are the weighted performance measures, WLS seems to outperform. Still, we can say that when heteroscedasticity does not exist, weighted measures are misleading because errors are weighted in inverse proportion of the sample variances although they should be weighted equally. On the other hand, OLS (variance-covariance matrix is known/unknown) and MVR do not differ in terms of MSE and R^2 due to the estimated $\boldsymbol{\beta}$ values' being same. It is expected because when the responses are not correlated and the set of predictors for the responses is the same, OLS and MVR are equivalent. Even if correlation exists, OLS and MVR produce the same estimates for $\boldsymbol{\beta}$, but with a different prediction variance.

Considering d_{H}, we observe that OLS estimates the true distribution of a single observation at some design (center or corner) point better than the other methods. When variance-covariance matrix is known, it even estimates better. Estimation of MVR is very close to OLS and it gets closer when the number of replications is increased. On the other hand, WLS estimation is the worst, and it is far from the true distribution. Considering the confidence and prediction regions, we can make similar observations to those of d_{H}. WLS gives very narrow prediction regions However, the main reason of this is that weighted MSE is not a good estimator of true error variation at any specified design point.

Generally, methods perform better at the center points which is expected because estimation and prediction errors are higher outside the center of the design region when the error variance is homogeneous.

4.2 Scenarios 3-4: WLS Case

WLS is applicable when the responses are not correlated and the error variances are not homogeneous. True mean, variance and covariance values at each design point of the experimental design for this case, which are all predetermined, are given in Table B.1 in Appendix B. Data in scenarios 3 and 4 are generated accordingly. WLS is applicable for both of the scenarios. The only difference between these scenarios is the number of replications. We make an analysis by choosing different number of replications (n=5 and n=25) and try to observe the effect of number of replications in the quality of the predictions. Generated data is given in Table B.2 for scenario 3 and in Table B.3 for scenario 4. After the data are generated, second-order response surface models are fitted to the responses by applying all regression methods under consideration, and performances of them are analyzed. Estimated model coefficients and predictions made at the center and the corner points of the designed experiment are given in Table B.4 through Table B.9.

Table 4.7 Performance measures (scenario 3)

Performance Measures	WLS (Variance Known)	OLS	WLS	MVR
trace[Cov($\hat{\boldsymbol{\beta}}$)]	1.355	2.249	0.714	2.024
det[Cov($\hat{\boldsymbol{\beta}}$)]	410.732x10^{-47}	57.853x10^{-24}	0.036x10^{-47}	4.238x10^{-24}
MSE_1	9.416 (0.927)	9.110	9.555 (1.170)	9.110
MSE_2	2.567 (0.757)	2.478	2.583 (0.975)	2.478
R_1^2	0.938 (0.999)	0.940	0.937 (0.999)	0.940
R_2^2	0.903 (0.999)	0.906	0.902 (0.998)	0.906

Table 4.8 Performance measures at the center point (scenario 3)

Performance Measures	WLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.663	0.303	0.284	0.273
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.244	0.082	0.174	0.074
d_{H}	0.160	0.489	0.938	0.547

Table 4.9 Performance measures at the corner point (scenario 3)

Performance Measures	WLS (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.053	1.221	0.031	1.099
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.052	0.332	0.024	0.299
d_{H}	0.261	0.993	0.506	0.965

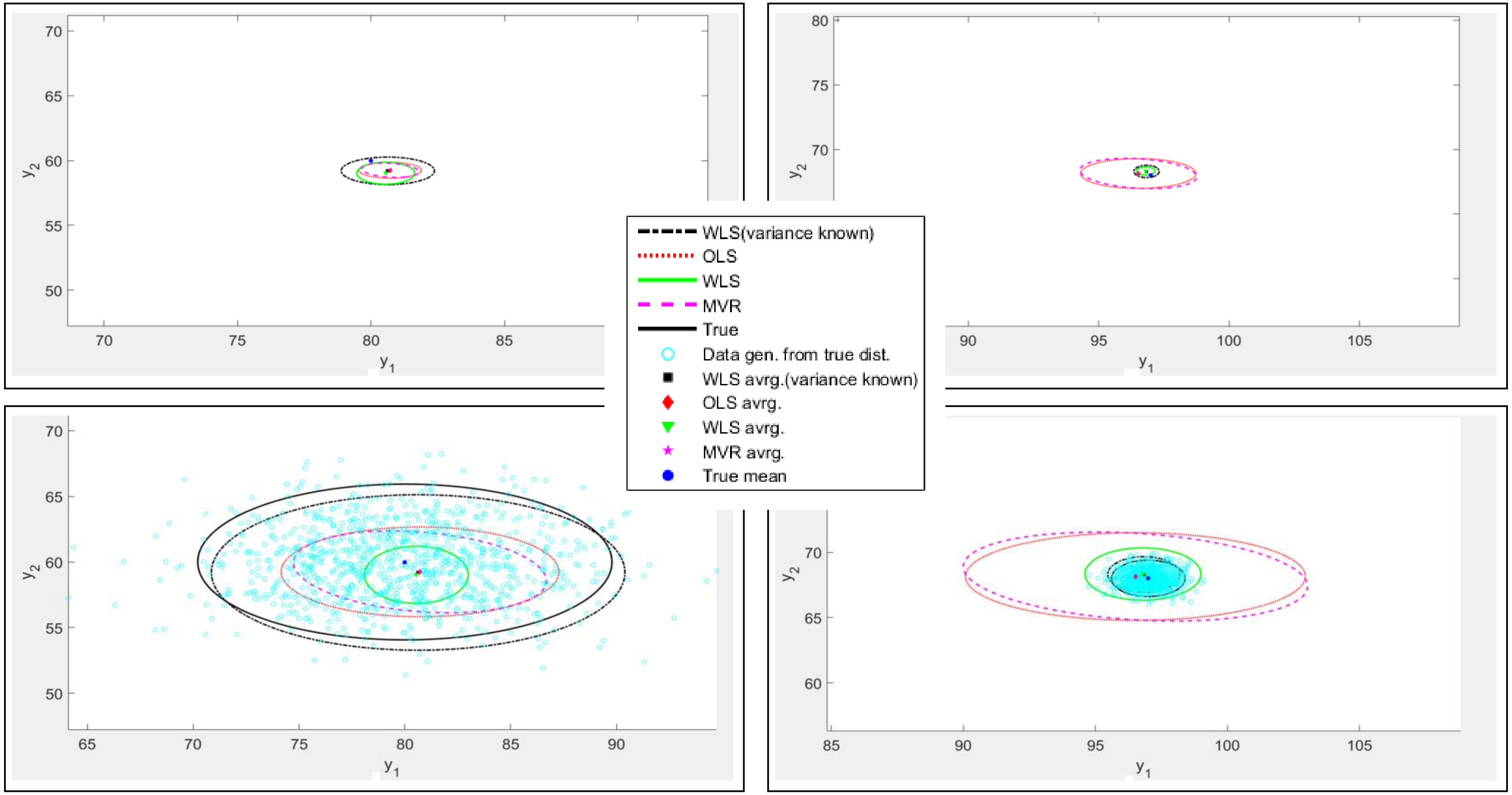

Figure 4.3 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 3)

Table 4.10 Performance measures (scenario 4)

Performance Measures	**WLS (Variance Known)**	**OLS**	**WLS**	**MVR**
trace[Cov($\hat{\boldsymbol{\beta}}$)]	0.271	0.417	0.243	0.409
det[Cov($\hat{\boldsymbol{\beta}}$)]	43.068x10^{-60}	3.977x10^{-37}	1.350x10^{-60}	2.635x10^{-37}
MSE_1	8.207 (0.913)	8.054	8.22 (1.018)	8.054
MSE_2	2.692 (0.856)	2.687	2.692 (1.001)	2.687
R_1^2	0.940 (0.999)	0.941	0.940 (0.999)	0.941
R_2^2	0.891 (0.996)	0.891	0.891 (0.996)	0.891

Table 4.11 Performance measures at the center point (scenario 4)

Performance Measures	**WLS (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.133	0.054	0.125	0.053
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.049	0.018	0.039	0.018
d_{H}	0.057	0.465	0.957	0.474

Table 4.12 Performance measures at the corner point (scenario 4)

Performance Measures	**WLS (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.011	0.216	0.012	0.212
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.010	0.072	0.010	0.071
d_{H}	0.022	0.989	0.473	0.984

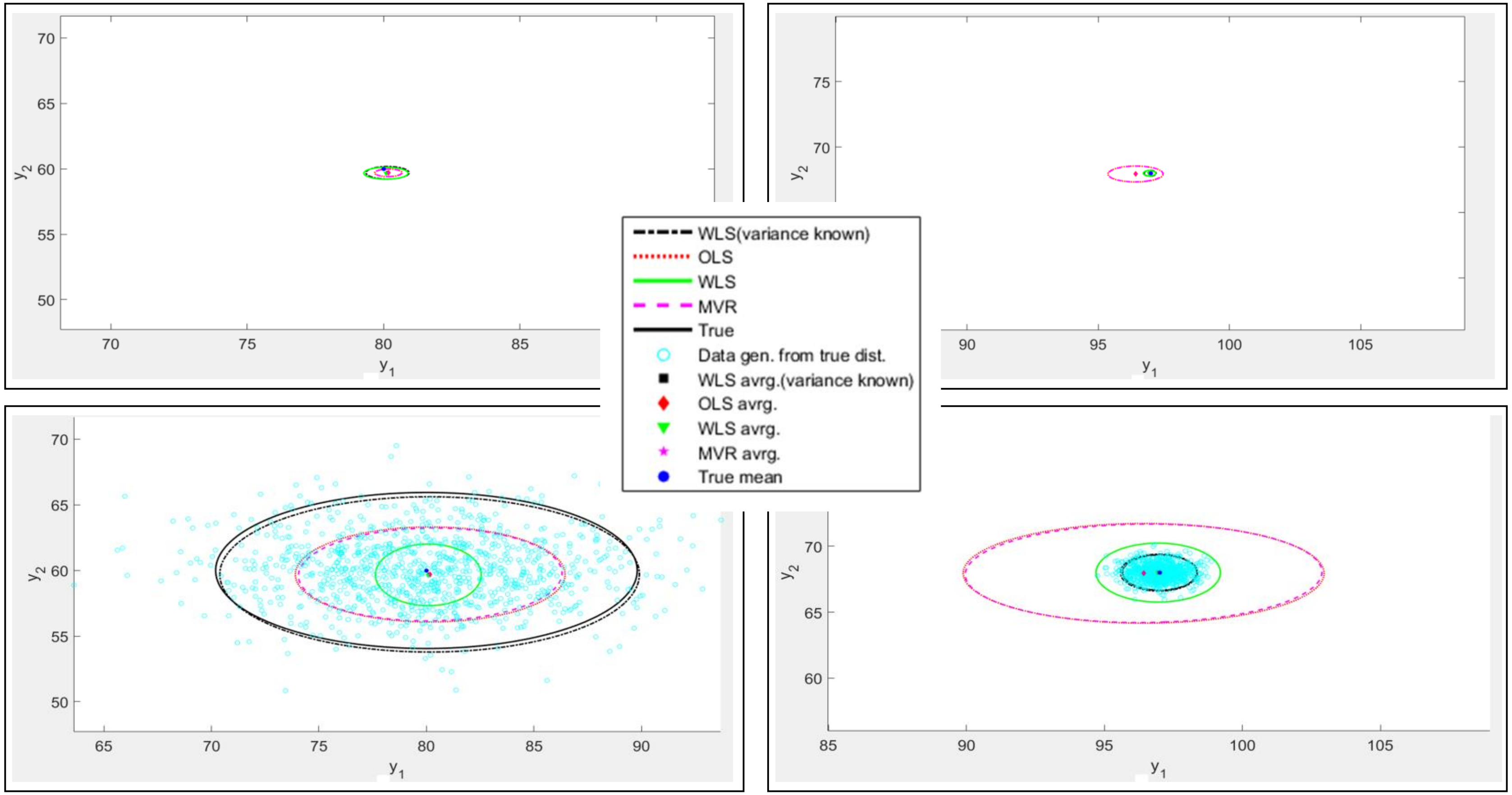

Figure 4.4 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 4)

Scenarios 3 and 4 have the circumstances that WLS is appropriate for use, further WLS is known as BLUE if the variance-covariance matrix of the error terms is known. We observe that WLS, no matter variance-covariance matrix is known or not, seems to outperform in terms of the spread of the estimated parameters, i.e. it estimates $\boldsymbol{\beta}$ with lower values of trace[Cov($\widehat{\boldsymbol{\beta}}$)] and det[Cov($\widehat{\boldsymbol{\beta}}$)]. Especially, det[Cov($\widehat{\boldsymbol{\beta}}$)] is lower a lot more in WLS. However, when it uses the estimate of variance-covariance matrix in scenario 3, it seems much better than it is. However, in scenario 4, since the number of replications is increased, variance-covariance matrices used are estimated more accurately, and so performances of the WLS with and without known variance-covariance matrix get closer. MVR seems slightly better than OLS; however, this might be due to randomness. Variance-covariance matrix used in MVR see a small correlation in the sample data, so it affects the variance of estimated $\boldsymbol{\beta}$, but not the estimated $\boldsymbol{\beta}$ itself. When the set of predictors for the responses is the same, OLS and MVR produce the same estimates for $\boldsymbol{\beta}$, but with a different prediction variance depending on the existence of correlation.

At the center point, OLS and MVR predict mean responses $\widehat{\mathrm{E}}(y_1)$ and $\widehat{\mathrm{E}}(y_2)$ with smaller variances than WLS. At the corner point, however, WLS is much better than OLS and MVR. Moreover, WLS performs better at the corner point rather than the center point in contrast to OLS and MVR. Then, we can conclude that performance of WLS in terms of the variances of the predicted mean responses depends on the position of the design point. Further, we may say that WLS performs better when the true error variance is small at the selected design point, which is the corner point in this particular example. Additionally, performance of WLS in terms of the variances of the predicted mean responses depends on the number of replications. Its performance is better when the number of replications is high, which is expected.

Considering MSE and R^2 in parentheses, which are the weighted performance measures and valid for scenario 3 and 4 because heteroscedasticity exists, WLS is much better than OLS and MVR. WLS gives weights to each observation so that observations with large variances have less influence in determining the model parameters while the observations with small variances have more. Thus, while evaluating the error in prediction, we should give more weights to the observations with smaller variances. OLS and MVR give same values for MSE and R^2 since they produce the same estimates for $\boldsymbol{\beta}$ (but with different variances). R^2 values of the responses given in parentheses are very high, which may be interpreted as an indicator of an overfitting problem. However, this can be expected aside from overfitting since the true mean functions are also second-order polynomials as the fitted models and adjusted R^2 values of these models are also 0.99.

Considering d_{H}, we observe that WLS estimates the true distribution of a single observation much better than the other methods when variance-covariance matrix is known. However, when it is not known, it may not perform so well depending on the position of the design point. For example, when variance-covariance matrix is unknown, it still estimates closer to the true distribution at the corner point, but not at the center point. This might be because of the fact that weighted MSE provides a good estimate of the true error variance at the corner point while for some other points it does not. Estimates made by OLS and MVR seem to have similar distances from the true distribution. Their performance gets worse even more at the corner point as expected. Additionally, when the number of replications is high, we observe improvement in d_{H} for all methods.

Considering the confidence and prediction regions, we can make similar conclusions. WLS produces better confidence regions (using the confidence region by BLUE as base), especially when the number of replications is high and/or variance-covariance matrix is known. Also, depending on the position of the design point, its performance gets even better than other methods. For example, we observe that confidence region of WLS is much better at the corner point.

At the center point, all methods give narrow prediction regions when the variance-covariance matrix is not known, and WLS gives much narrower ones. On the other hand, at the corner point, all methods give larger prediction regions, and OLS and

MVR give much larger ones. This is because the methods estimate true error variances as defined previously, but this estimation is not done according to the design point. We simply use MSE values. Thus, true error variances are underestimated at some points, and overestimated at other points. In other words, prediction regions seem to highly depend on the estimation of true error variances at the specified design point. In order to improve prediction regions of the methods, some other estimators of true error variance can be used. If the variance-covariance matrix is known, heteroscedasticity exists and there is no correlation, prediction region by WLS is the closest to the true region.

4.3 Scenarios 5-8: MVR Case

MVR is applicable when the responses are correlated, the error variances are homogeneous and sets of predictors of the responses are the same. True mean, variance and covariance values at each design point of the experimental design for this case, which are all predetermined, are given in Table C.1 in Appendix C for scenarios 5 and 6, and in Table C.2 for scenarios 7 and 8. MVR is applicable for all of these scenarios. SUR is also applicable, but it is actually equivalent to MVR since the set of the predictors of the responses are the same. The difference between these scenarios is due to the number of replications and value of the correlation coefficient. We make an analysis by choosing different number of replications (n=5 and n=25) and try to observe the effect of number of replications in the quality of the predictions. We also try some low (0.30) and high (0.90) values of correlation coefficients to draw conclusions about the behavior of the methods while correlation increases. Generated data are given in Table C.3 through Table C.6. After the data are generated, second-order response surface models are fitted to the responses by applying all regression methods under consideration, and performances of them are analyzed. Estimated model coefficients and predictions made at the center and the corner points of the designed experiment are given in Table C.7 through Table C.18.

Table 4.13 Performance measures (scenario 5)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
trace[Cov($\widehat{\boldsymbol{\beta}}$)]	5.332	4.533	3.646	4.079
det[Cov($\widehat{\boldsymbol{\beta}}$)]	339.665x10^{-17}	5.365x10^{-17}	0.014x10^{-17}	0.594x10^{-17}
MSE_1	18.548	18.548	18.924 (1.182)	18.548
MSE_2	4.809	4.809	4.890 (1.028)	4.809
R_1^2	0.883	0.883	0.881 (0.885)	0.883
R_2^2	0.839	0.839	0.836 (0.881)	0.839

Table 4.14 Performance measures at the center point (scenario 5)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.668	0.617	0.285	0.555
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.246	0.160	0.089	0.144
d_{H}	0.159	0.256	0.938	0.264

Table 4.15 Performance measures at the corner point (scenario 5)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	2.692	2.486	1.605	2.237
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.990	0.645	0.537	0.580
d_{H}	0.242	0.308	0.854	0.319

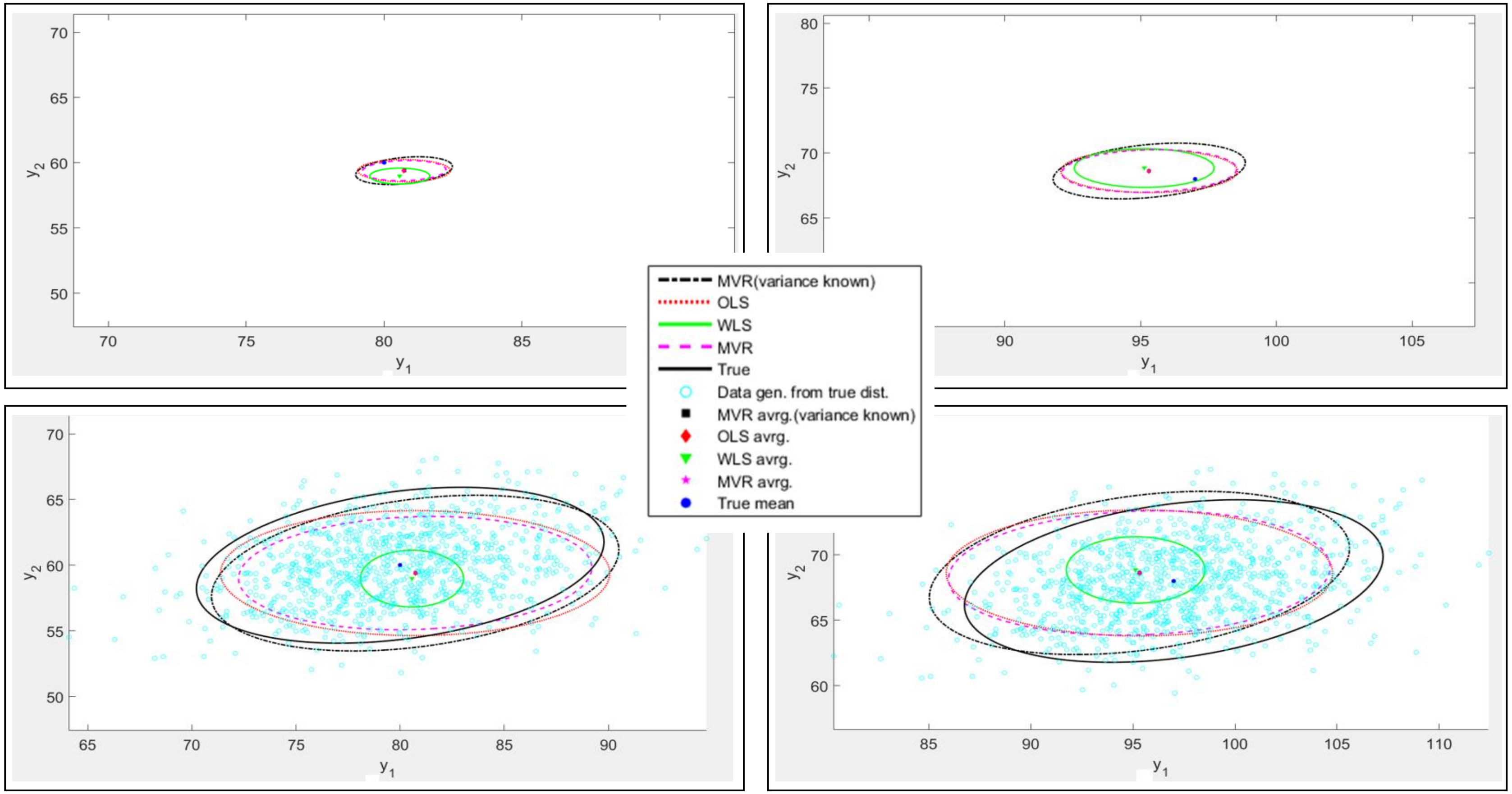

Figure 4.5 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 5)

Table 4.16 Performance measures (scenario 6)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
trace[Cov($\hat{\boldsymbol{\beta}}$)]	1.066	0.949	0.926	0.930
det[Cov($\hat{\boldsymbol{\beta}}$)]	35.616x10^{-30}	6.736x10^{-30}	2.144x10^{-30}	1.889x10^{-30}
MSE_1	18.167	18.167	18.177 (1.004)	18.167
MSE_2	6.294	6.294	6.295 (1.004)	6.294
R_1^2	0.871	0.871	0.871 (0.881)	0.871
R_2^2	0.772	0.772	0.772 (0.785)	0.772

Table 4.17 Performance measures at the center point (scenario 6)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.134	0.121	0.126	0.118
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.049	0.042	0.042	0.041
d_{H}	0.063	0.171	0.950	0.099

Table 4.18 Performance measures at the corner point (scenario 6)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.538	0.487	0.555	0.477
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.198	0.169	0.201	0.165
d_{H}	0.058	0.172	0.897	0.096

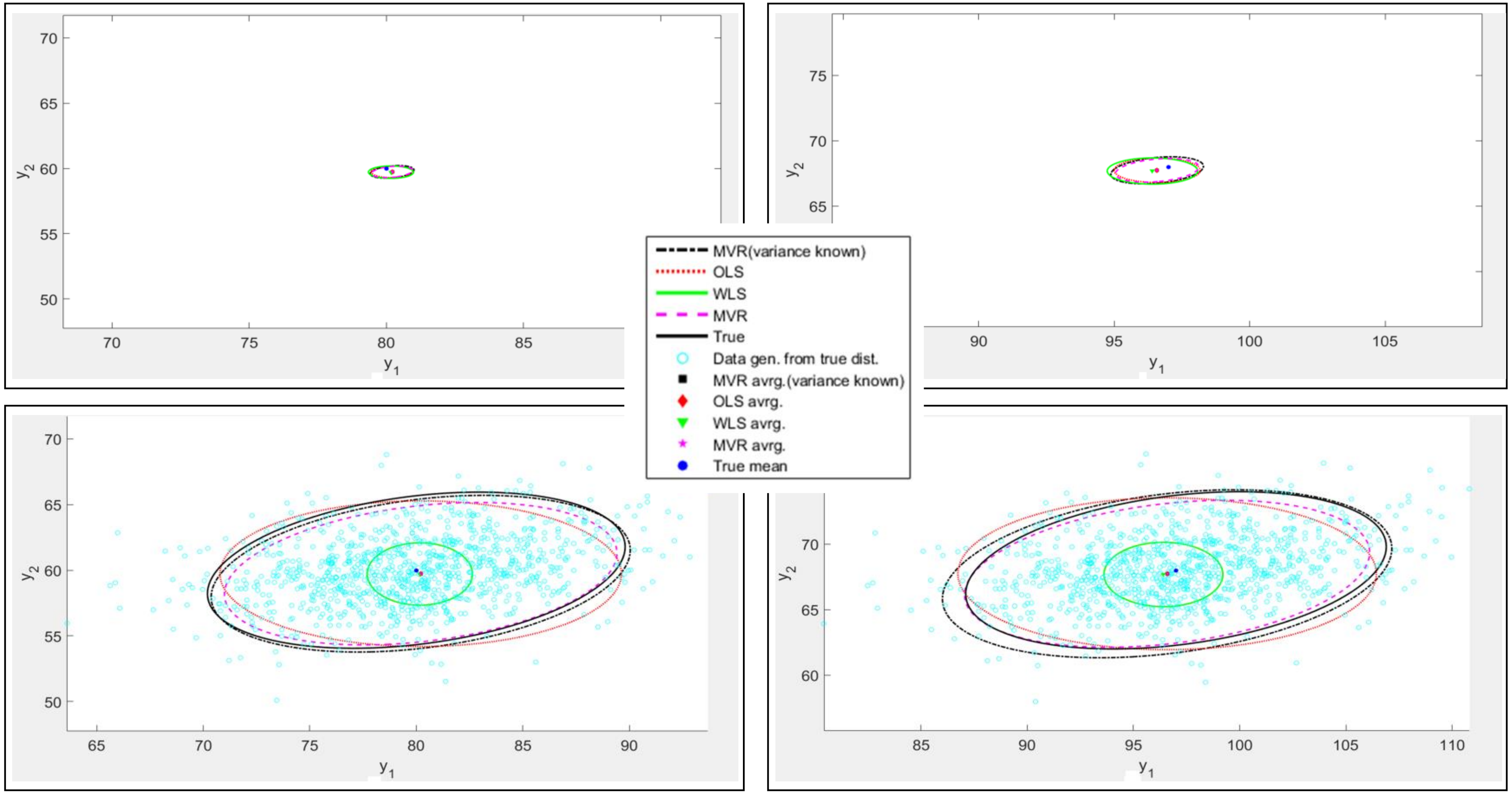

Figure 4.6 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 6)

Table 4.19 Performance measures (scenario 7)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
trace[Cov($\hat{\boldsymbol{\beta}}$)]	5.332	4.640	3.784	4.176
det[Cov($\hat{\boldsymbol{\beta}}$)]	534.777x10^{-24}	159.338x10^{-18}	0.160x10^{-18}	0.932x10^{-24}
MSE_1	18.548	18.548	18.924 (1.182)	18.548
MSE_2	5.362	5.362	5.689 (1.276)	5.362
R_1^2	0.883	0.883	0.881 (0.885)	0.883
R_2^2	0.827	0.827	0.816 (0.933)	0.827

Table 4.20 Performance measures at the center point (scenario 7)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.668	0.617	0.285	0.555
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.246	0.178	0.144	0.161
d_{H}	0.159	0.705	0.829	0.265

Table 4.21 Performance measures at the corner point (scenario 7)

Performance Measures	MVR (Variance Known)	OLS	WLS	MVR
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	2.692	2.486	1.605	2.237
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.990	0.719	0.574	0.647
d_{H}	0.242	0.718	0.795	0.320

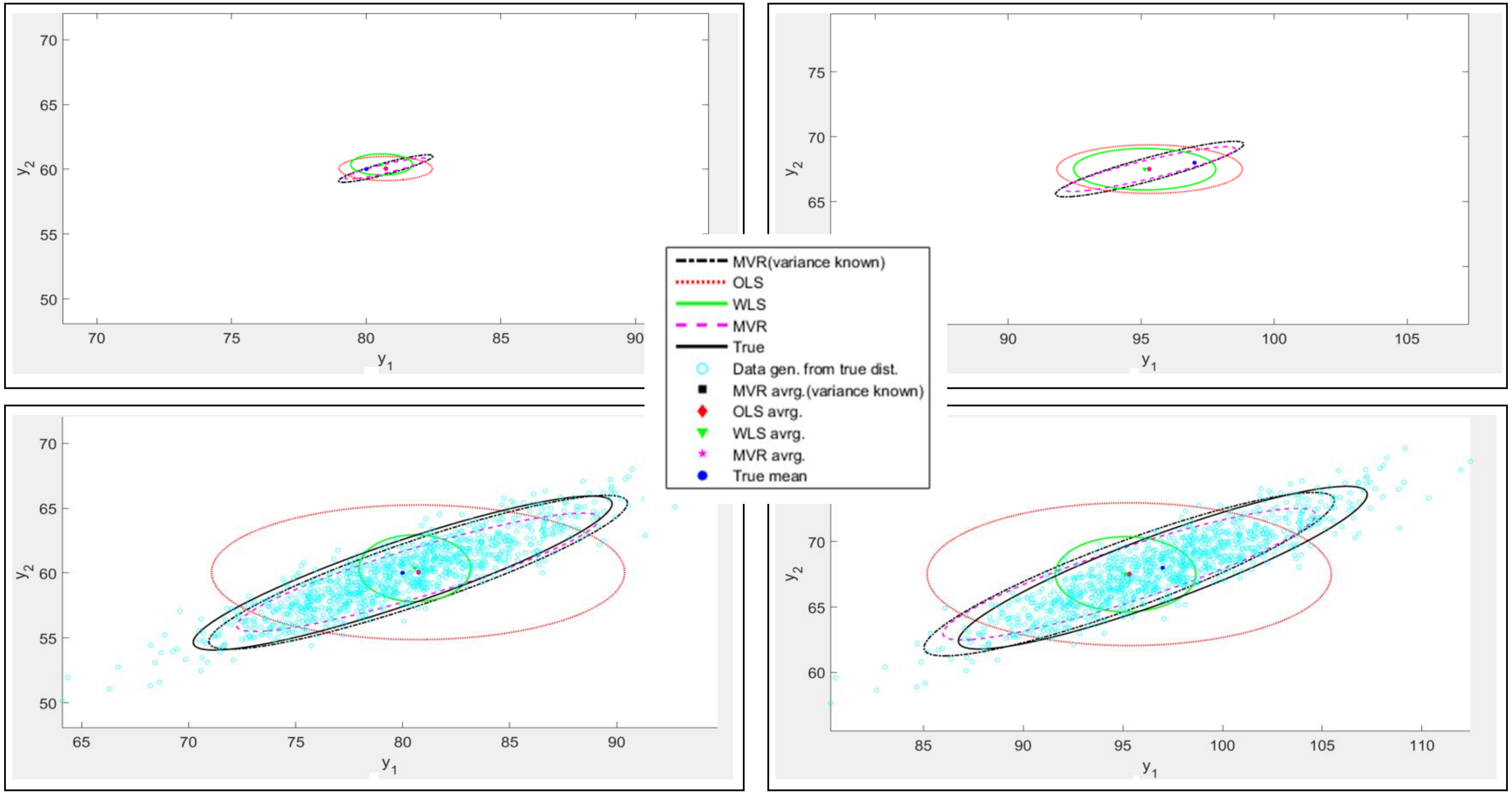

Figure 4.7 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 7)

Table 4.22 Performance measures (scenario 8)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
trace[Cov($\widehat{\boldsymbol{\beta}}$)]	1.066	0.958	0.930	0.938
det[Cov($\widehat{\boldsymbol{\beta}}$)]	56.075x10^{-37}	9.408x10^{-30}	2.180x10^{-18}	2.971x10^{-37}
MSE_1	18.167	18.167	18.176 (1.004)	18.167
MSE_2	6.508	6.508	6.513 (1.001)	6.508
R_1^2	0.871	0.871	0.871 (0.8813)	0.871
R_2^2	0.755	0.755	0.754 (0.795)	0.755

Table 4.23 Performance measures at the center point (scenario 8)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.134	0.121	0.126	0.118
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.049	0.043	0.048	0.042
d_{H}	0.063	0.709	0.865	0.099

Table 4.24 Performance measures at the corner point (scenario 8)

Performance Measures	**MVR (Variance Known)**	**OLS**	**WLS**	**MVR**
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.538	0.487	0.555	0.477
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.198	0.174	0.205	0.171
d_{H}	0.058	0.710	0.829	0.096

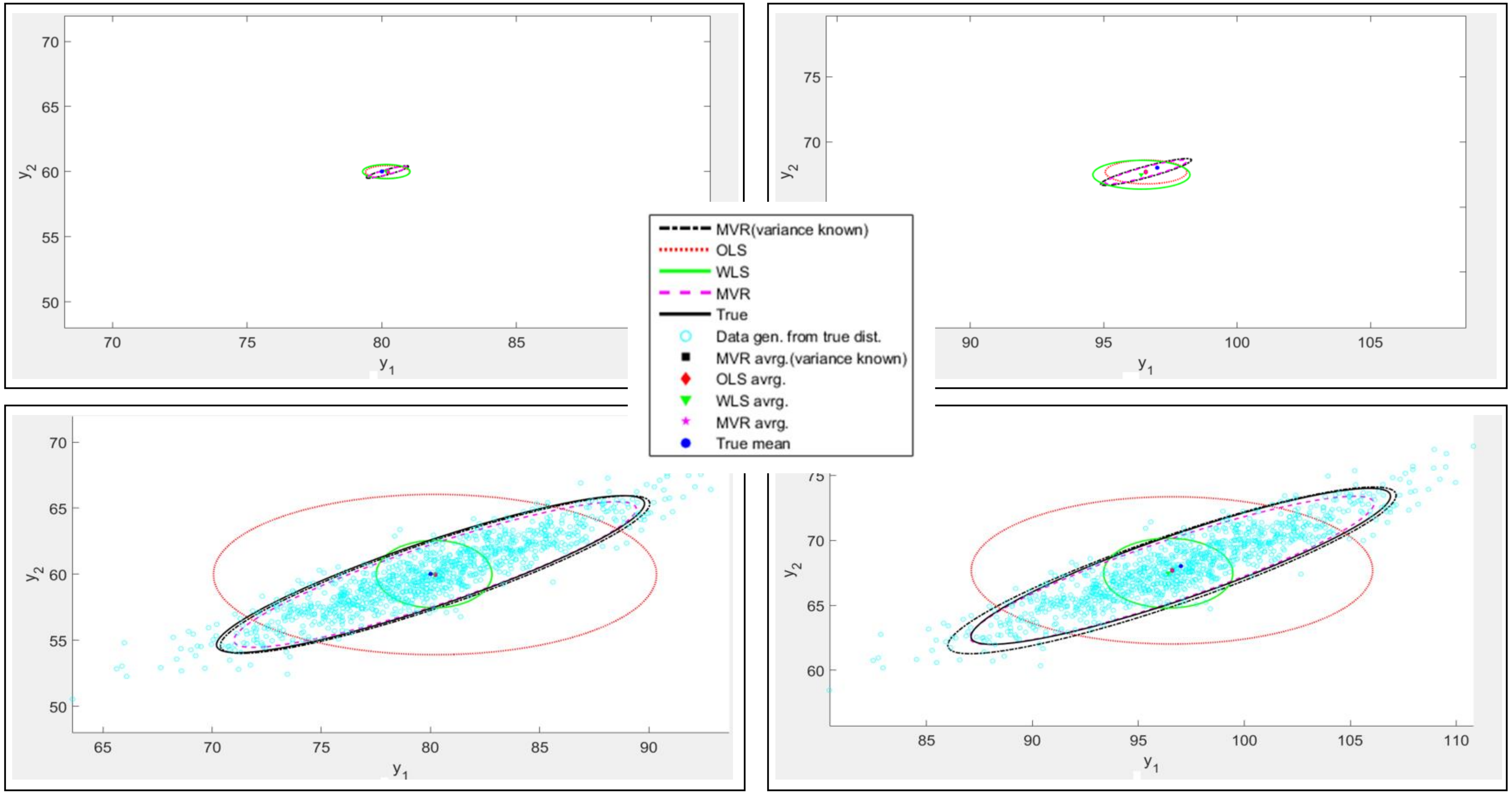

Figure 4.8 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 8)

Scenarios from 5 to 8 are generated considering MVR assumptions under which MVR is BLUE if the variance-covariance matrix is known. For each of these scenarios, OLS and MVR (either variance-covariance matrix is known or unknown) estimate $\boldsymbol{\beta}$ the same. They differ by their spread or efficiency, i.e. variance-covariance matrix of estimated $\boldsymbol{\beta}$. Thus, for each of the scenarios here MSE and R^2 are the same for OLS and MVR, and for WLS is not so much different. However, according to the weighted performance measures in parenthesis given for WLS, WLS is the best by landslide, which is a misleading situation since weights are given to the observations according to the sample variances which are statistically not different from each other.

We expect that gain in the efficiency in the parameter estimation to be higher when correlation between responses are high and when we use MVR. Although we cannot observe this expectation completely in terms of trace[Cov($\widehat{\boldsymbol{\beta}}$)], det[Cov($\widehat{\boldsymbol{\beta}}$)] is in accordance with it. det[Cov($\widehat{\boldsymbol{\beta}}$)] obtained by using MVR is much lower than those obtained by other methods in scenario 7 and 8. Further, gain in the efficiency increases much more when the number of replications is increased. We also observe that when methods use estimated variance-covariance matrix, their performance can be better than it really is. However, this cannot be a conclusion since it might be due to the randomness in data. Still, when the number of replications, i.e. accuracy in estimation of the variance-covariance matrix, is increased, their performances get much closer to each other.

Considering d_{H}, we observe that MVR estimates the true distribution of a single observation at design point selected much better than the other regression methods especially when the number of replications and/or correlation between responses are high. OLS estimates the true distribution with a close performance to MVR if the number of replications and correlation are low, otherwise it is worse. WLS always seems to make a prediction far from the true distribution, which is again due to the fact that weighted MSE is not a good estimator of true error variation at specified design points for these particular scenarios.

We observe that methods perform better at the center points than at the corner points, i.e. estimation error in mean responses seems to be lower.

Considering the confidence and prediction regions, WLS always produces very small regions compared to OLS and MVR. When both of the correlation and number of replications are low, regions of OLS and MVR do not differ much. When the correlation is low, but the number of replications is high they slightly differ. When the correlation is high, MVR captures it and presents totally different regions. WLS and OLS give larger confidence regions unnecessarily. OLS also gives larger prediction regions and still cannot cover the observations well. On the other hand, WLS has too small prediction regions. However, prediction regions of MVR are very close to the true prediction in scenarios through 5 to 8.

4.4 Scenarios 9-12: SUR Case

SUR is applicable when the responses are correlated and the error variances are homogeneous. Sets of predictors of the responses are not necessarily the same. True mean, variance and covariance values at each design point of the experimental design for this case, which are all predetermined, are given in Table D.1 in Appendix D for scenarios 9 and 10, and in Table D.2 for scenarios 11 and 12. SUR is applicable for all of these scenarios. Difference between these scenarios is due to the number of replications and the value of correlation coefficient. We make analysis by choosing different number of replications (n=5 and n=25) and try to observe the effect of number of replications in the quality of the predictions. We also try some low (0.30) and high (0.90) values of correlation coefficients to draw conclusions about the behavior of the methods while the correlation increases. Generated data are given in Table D.3 through Table D.6. After the data are generated, second-order response surface models are fitted to the responses by applying all regression methods under consideration, and performances of them are analyzed. Estimated model coefficients and predictions made at the center and the corner points of the designed experiment are given in Table D.7 through Table D.18.

Table 4.25 Performance measures (scenario 9)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
trace[Cov($\widehat{\boldsymbol{\beta}}$)]	3.908	3.787	3.091	3.398
det[Cov($\widehat{\boldsymbol{\beta}}$)]	467.840x10^{-11}	145.329x10^{-11}	4.949x10^{-11}	42.340x10^{-11}
MSE_1	18.628	18.548	18.924 (1.182)	18.559
MSE_2	4.765	4.765	4.877 (1.140)	4.765
R_1^2	0.883	0.883	0.881 (0.885)	0.883
R_2^2	0.789	0.789	0.784 (0.810)	0.789

Table 4.26 Performance measures at the center point (scenario 9)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.626	0.617	0.285	0.552
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.074	0.048	0.030	0.046
d_{H}	0.126	0.230	0.914	0.222

Table 4.27 Performance measures at the corner point (scenario 9)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	2.521	2.486	1.605	2.224
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.291	0.187	0.149	0.182
d_{H}	0.220	0.270	0.846	0.274

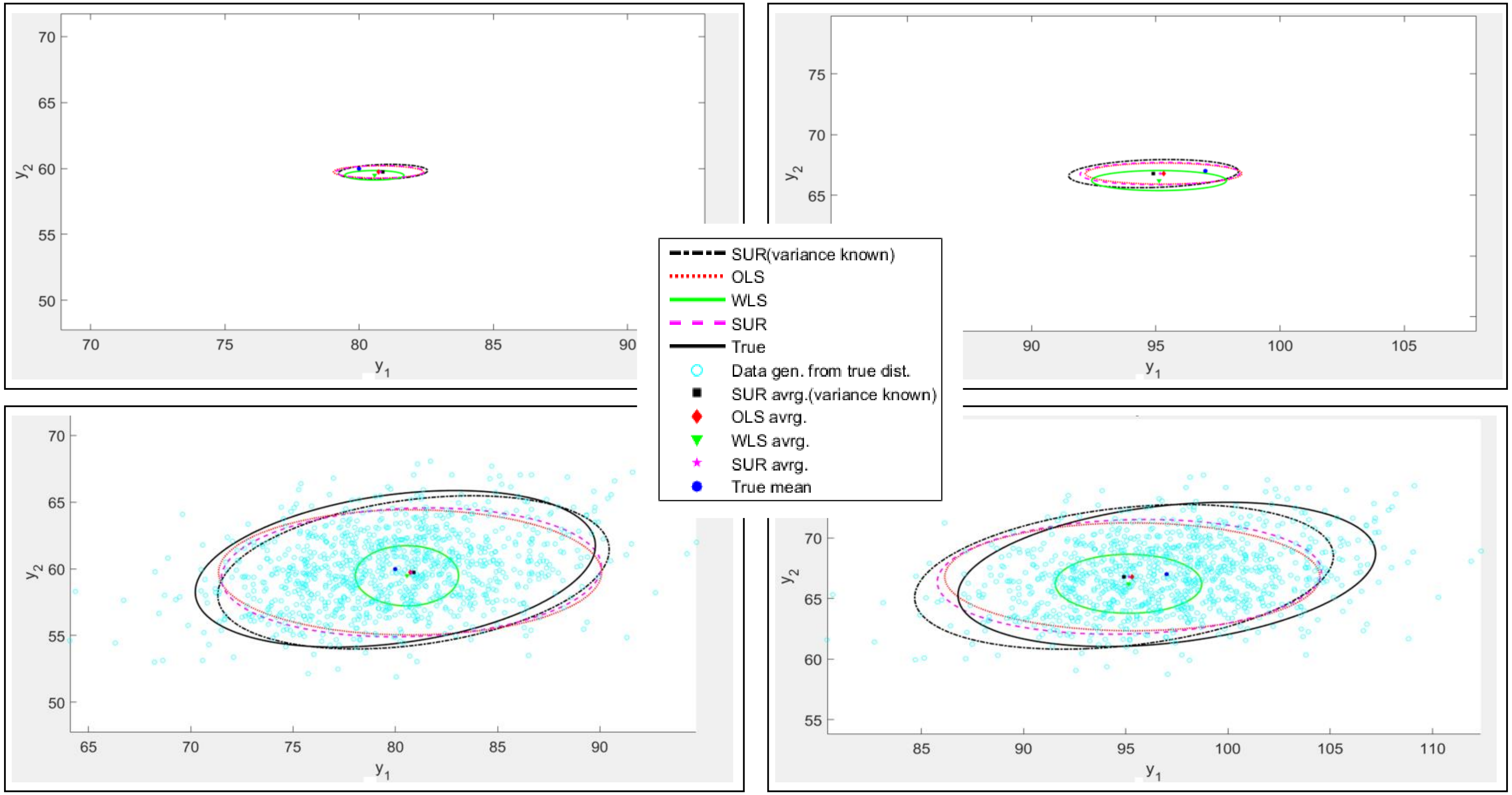

Figure 4.9 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 9)

Table 4.28 Performance measures (scenario 10)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
trace[Cov($\hat{\boldsymbol{\beta}}$)]	0.782	0.755	0.729	0.695
det[Cov($\hat{\boldsymbol{\beta}}$)]	38.325x10^{-19}	22.476x10^{-19}	8.963x10^{-19}	7.693x10^{-19}
MSE_1	18.193	18.167	18.176 (1.004)	18.192
MSE_2	6.312	6.312	6.313 (1.008)	6.312
R_1^2	0.871	0.871	0.871 (0.881)	0.871
R_2^2	0.731	0.731	0.731 (0.733)	0.731

Table 4.29 Performance measures at the center point (scenario 10)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.125	0.121	0.126	0.112
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.015	0.013	0.012	0.013
d_{H}	0.051	0.165	0.951	0.087

Table 4.30 Performance measures at the corner point (scenario 10)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.504	0.487	0.555	0.450
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.058	0.050	0.052	0.049
d_{H}	0.045	0.167	0.909	0.084

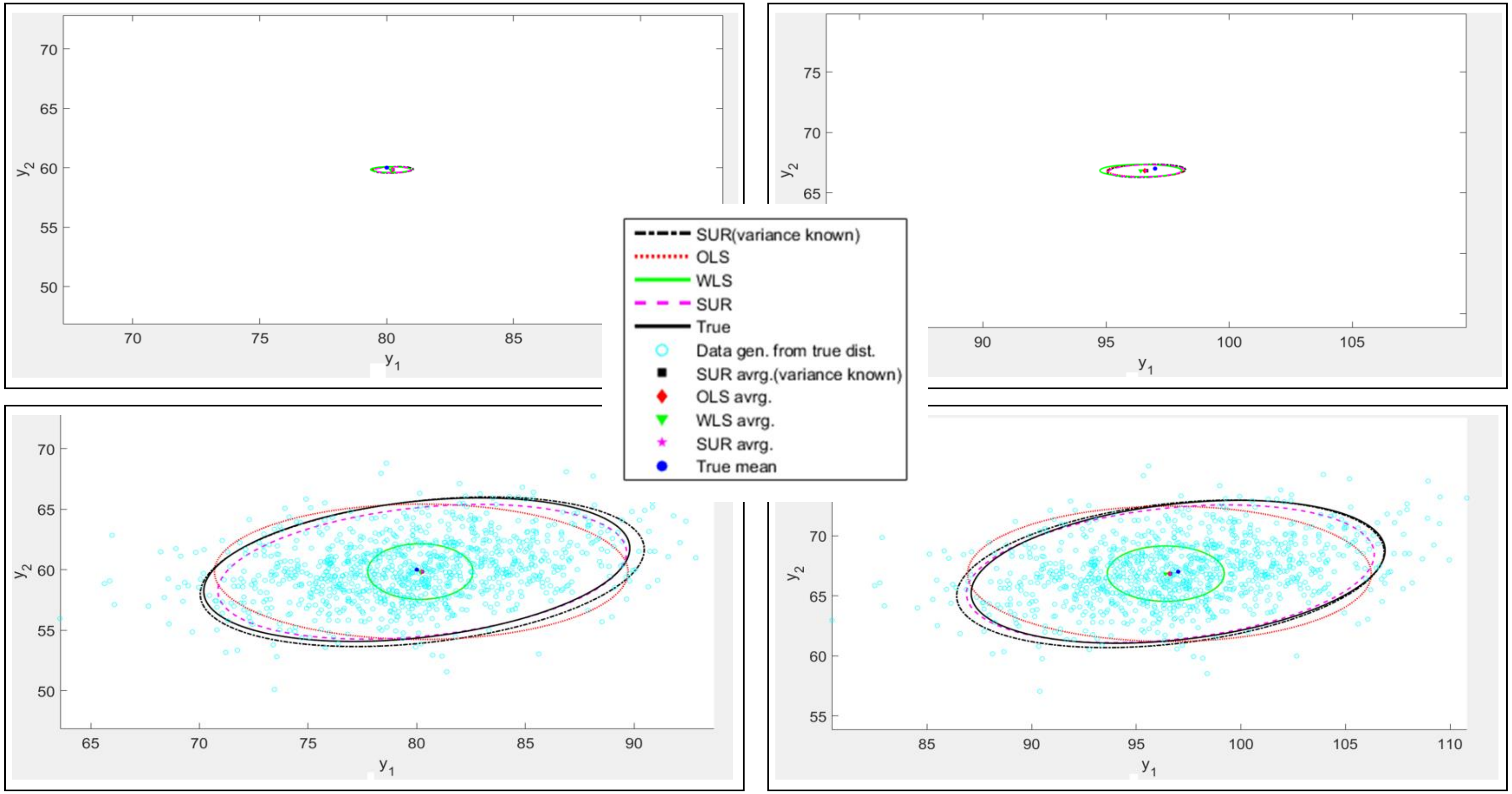

Figure 4.10 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 10)

Table 4.31 Performance measures (scenario 11)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
trace[Cov($\hat{\boldsymbol{\beta}}$)]	1.671	3.808	3.055	1.468
det[Cov($\hat{\boldsymbol{\beta}}$)]	7.366x10^{-16}	200.299x10^{-11}	1.754x10^{-11}	3.385x10^{-16}
MSE_1	19.326	18.548	18.924 (1.182)	19.424
MSE_2	5.303	5.303	5.422 (1.292)	5.303
R_1^2	0.878	0.883	0.881 (0.885)	0.878
R_2^2	0.781	0.781	0.777 (0.8824)	0.781

Table 4.32 Performance measures at the center point (scenario 11)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	0.290	0.617	0.285	0.258
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.074	0.053	0.037	0.051
d_{H}	0.159	0.703	0.831	0.209

Table 4.33 Performance measures at the corner point (scenario 11)

Performance Measures	**SUR (Variance Known)**	**OLS**	**WLS**	**SUR**
$\mathrm{Var}(\hat{\mathrm{E}}(y_1))$	1.151	2.486	1.605	1.029
$\mathrm{Var}(\hat{\mathrm{E}}(y_2))$	0.291	0.208	0.146	0.202
d_{H}	0.229	0.719	0.877	0.255

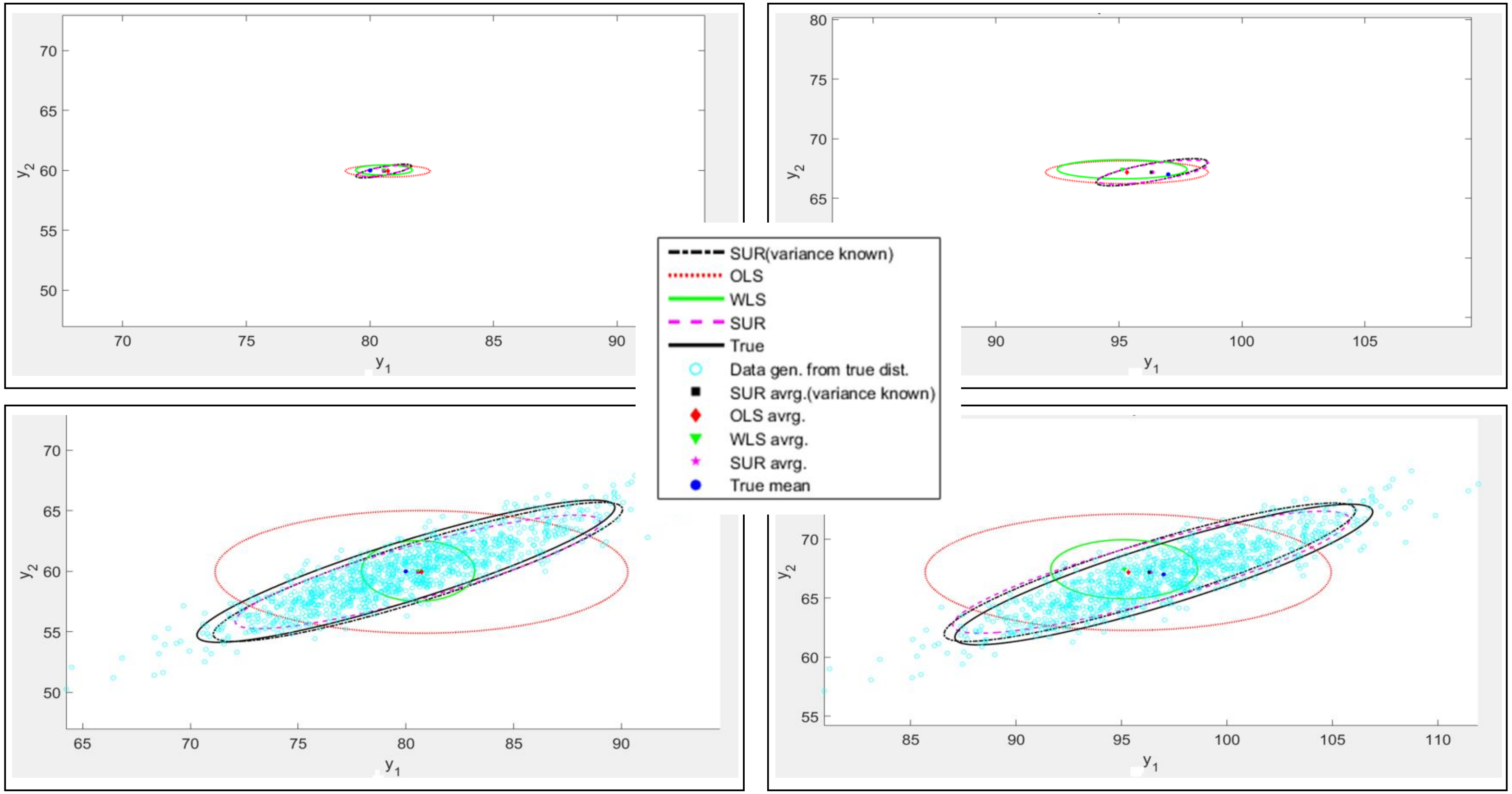

Figure 4. 11 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 11)

Table 4.34 Performance measures (scenario 12)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
trace[Cov($\widehat{\boldsymbol{\beta}}$)]	0.334	0.757	0.729	0.306
det[Cov($\widehat{\boldsymbol{\beta}}$)]	6.034×10^{-25}	25.671×10^{-19}	8.655×10^{-11}	3.063×10^{-25}
MSE_1	18.573	18.167	18.176 (1.004)	18.564
MSE_2	6.598	6.598	6.601 (1.019)	6.598
R_1^2	0.868	0.871	0.871 (0.881)	0.869
R_2^2	0.710	0.710	0.710 (0.740)	0.710

Table 4.35 Performance measures at the center point (scenario 12)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.058	0.121	0.126	0.053
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.015	0.013	0.012	0.013
d_{H}	0.067	0.709	0.869	0.082

Table 4.36 Performance measures at the corner point (scenario 12)

Performance Measures	SUR (Variance Known)	OLS	WLS	SUR
$\mathrm{Var}(\widehat{\mathrm{E}}(y_1))$	0.230	0.487	0.555	0.210
$\mathrm{Var}(\widehat{\mathrm{E}}(y_2))$	0.058	0.052	0.046	0.052
d_{H}	0.064	0.709	0.830	0.079

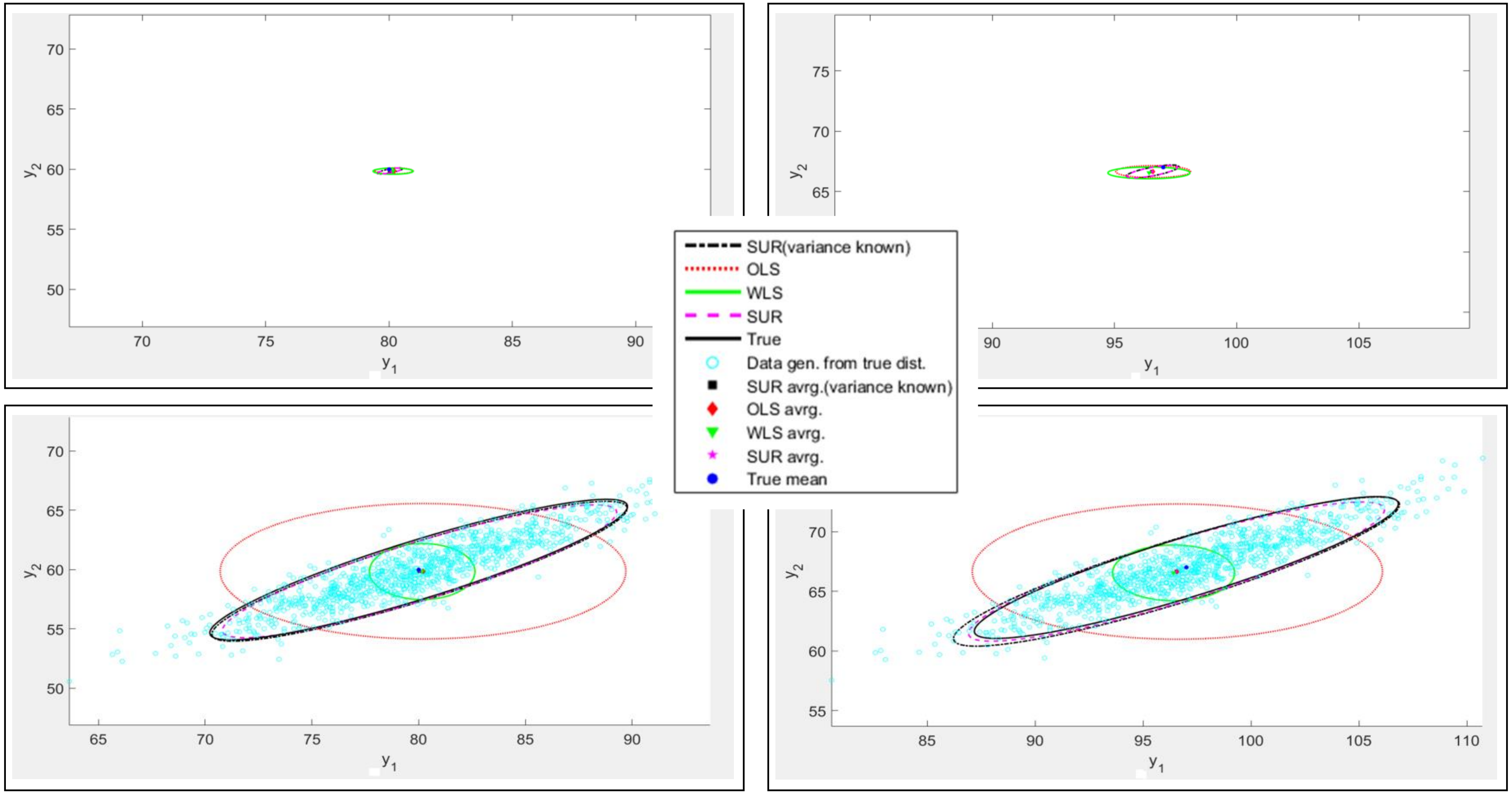

Figure 4.12 Confidence (at top) and prediction (at bottom) regions for the center (on left) and the corner (on right) points (scenario 12)

Scenarios from 9 to 12 are generated considering SUR assumptions under which SUR is BLUE if the variance-covariance matrix is known. The only difference of these scenarios from the scenarios in MVR case is that the second response has a different set of significant predictors. Thus, SUR estimators of model parameters are different in their values from OLS estimators. Thus, MSE and R^2 are now different for these methods, but still they are very close. However, when correlation exists, SUR is capable of producing more efficient estimators of model parameters, which we observe through the results we obtain, as well. We observe maximum gain in the efficiency in the parameter estimation by SUR when correlation between responses and number of replications are high. This observation is the same as that we have in the previous heading. Further, we see that all comments we make in the previous heading are still valid here.

4.5 Statistical Analysis of Hellinger Distance Differences

Considering all scenarios together, we make a statistical analysis of the Hellinger distance results to draw conclusions about whether or not each method estimates the distribution of a single observation significantly different from that of the BLUE estimator. If so, we are also particularly interested in the factors which make the difference. Accordingly, we conduct ANOVA of differences between Hellinger distances of a method from that of the BLUE estimator for the scenarios. Analyzed data are given in Table E.1 in Appendix E, and the results obtained are provided in Tables E.2 through E.4. To satisfy the ANOVA assumptions a log transformation is applied to the difference data when it is necessary, and residual and main effects plots are shown in Figures E.1 through E.6.

We can make the following comments based on the ANOVA results: First comment is that, the difference between distance of BLUE and that of OLS on the average depends on whether OLS is applicable for that case or not. In the main effects plot in Figure E.2, it is seen that when OLS is not applicable, this difference is significantly larger than that when OLS is applicable. The difference also seems to depend on correlation between the responses and the number of replications. In

Figure E.2, we observe that when correlation is very high (0.9), the difference is significantly larger. Also, when the number of replications is high (n=25), the distance seems to be slightly larger, which is expected because of that BLUE does not necessarily correspond to the OLS in every scenario. When it does not, we expect the difference to be bigger when the number of replications is high. Otherwise, the difference is expected to be smaller.

On the average, the difference between distance of BLUE and that of WLS seems to significantly depend on the number of replications, heteroscedasticity, and position of the design point. This is similar to what we observe in the prediction region plots. It may be interesting to see that WLS applicability for the case is not a significant factor. This may be due to that even in the scenarios where WLS is applicable, WLS may perform poorly in terms of Hellinger distance depending on the design point and this seems due to the estimation of true error variation. We use weighted MSE as its estimator while applying WLS. We observe in the previous parts that this estimator does not work well at every design point. If another estimator were used for this variation, then we could expect WLS applicability to be a significant factor. Furthermore, we could expect WLS to outperform the others for the scenarios where WLS is applicable. Considering the main effects plot in Figure E.4, the difference between the distances of BLUE and WLS seems to be high when the number of replications is high (n=25), heteroscedasticity does not exist and position of the design point is the center, which we have already observed and discussed while analyzing the scenarios one by one.

Finally, the difference between distances of BLUE and that of SUR on the average seems to significantly depend on the number of the replications and heteroscedasticity. In Figure E.6, it is seen that the difference is small on the average when the number of replications is high (n=25) and there is no heteroscedasticity, which is expected. Correlation is not a significant factor for this difference because when correlation and heteroscedasticity do not exist, OLS is BLUE and SUR is already equivalent to OLS. When there is correlation and heteroscedasticity does not exist, SUR is already BLUE.

CHAPTER 5

CONCLUSION

In this study, we consider linear regression methods OLS, WLS, MVR and SUR typically used in MRDPO problems to fit response surface models to the data collected through statistically designed experiments. In MRDPO problems, it is assumed that each response has a non-homogeneous variance. Also, responses might be correlated. The methods we consider might not be appropriate for a particular MRDPO problem due to their restrictive assumptions. Thus, our interest in this study is to examine and compare these linear regression methods for their estimation and prediction errors. We are particularly interested in answering the following research question: Under which circumstances (violation of certain assumptions, being at a far point from the design center, number of replications etc.), estimation errors associated with model parameters and prediction errors associated with individual observations are high in MRDPO problems?

We base our conclusions on systematically generated scenarios on a typical MRDPO problem, and our observations of experimental results using certain performance measures and graphs of the confidence and prediction regions developed by a bootstrap approach.

First of all, we observe that OLS estimates the true distribution of a single observation at some design (center or corner) point better than the other methods only when it is applicable. When OLS is not applicable for a given scenario, difference between the distances of BLUE and OLS is considerable. We also observe that when correlation is high, the difference is considerably larger. Additionally, when the number of replications is high, the difference seems to be slightly larger, which is most probably due to that BLUE estimator estimates even better when the sample size is high and that BLUE does not necessarily correspond to the OLS in every scenario we consider.

Second, we observe that WLS, no matter variance-covariance matrix of error terms is known or not, seems to outperform the others in terms of the spread of the estimated parameters and model fit. Also, it estimates the true distribution of a single observation much better than the other methods when its assumptions are satisfied and variance-covariance matrix is known. However, when the variance-covariance matrix is not known, WLS may not perform so well depending on how well true error variation is estimated. Moreover, the difference between the distances of BLUE and WLS seems to significantly depend on the number of replications, heteroscedasticity, and position of the design point. When the number of replications is high, heteroscedasticity does not exist and position of the design point is where true error variance is high, WLS seems to be far from BLUE. Additionally, WLS might produce misleading results if its assumptions, which are heteroscedastic errors and uncorrelated responses, are not satisfied. In other words, when the assumptions are not satisfied, weighted performance measures (as those given by software such as Minitab and R) make us to consider we have good results in terms of model fit, but it may not be the true. However, it seems much better to use it when heteroscedasticity exists. Thus, WLS should be used when heteroscedasticity is highly expected as in MRDPO problems and there is no correlation of the responses or it is not high. Some statistical tests can be applied to data before applying WLS, but power of the tests is an important issue in that case.

When correlation among responses does not exist, OLS and MVR (SUR) perform similarly. However, when there is correlation and it is high, variances of the estimated model parameters, so the prediction variances and the distance from the true distribution get smaller in MVR (SUR). They all become much smaller when the number of replications is high. The difference between the distances of BLUE and SUR seems to significantly depend on the number of the replications and heteroscedasticity. It is seen that the difference is small on the average when sample size is high and there is no heteroscedasticity.

Observations obtained in this study is based on an experimental study. In order to generalize these observations, computational experiments can be expanded. As another future work, an appropriate linear regression method for the scenarios that have not been studied in this thesis can be searched. In these scenarios, not only heteroscedasticity should exist but also there should be correlation between responses. A regression method applicable for such scenarios is not readily available in the literature, or at least such a method has not been adopted for use in MRDPO problems, to the best of our knowledge. However, it would be very useful for both the product and process designers and researchers working in other fields of statistics and econometrics, since circumstances of these scenarios might be commonly encountered in these fields.

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APPENDIX A

GENERATED DATA AND MODEL PARAMETER ESTIMATES UNDER SCENARIOS 1-2: OLS CASE

Table A.1 True mean, variance and covariance values at experimental design points (scenarios 1&2)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	52.00	20.09	7.39	0
2	1	-1	-1	49.00	64.00	20.09	7.39	0
3	-1	1	-1	87.00	54.00	20.09	7.39	0
4	1	1	-1	69.00	62.00	20.09	7.39	0
5	-1	-1	1	71.00	58.00	20.09	7.39	0
6	1	-1	1	93.00	66.00	20.09	7.39	0
7	-1	1	1	67.00	64.00	20.09	7.39	0
8	1	1	1	97.00	68.00	20.09	7.39	0
9	-1.68	0	0	72.68	56.10	20.09	7.39	0
10	1.68	0	0	76.04	69.54	20.09	7.39	0
11	0	-1.68	0	81.75	61.14	20.09	7.39	0
12	0	1.68	0	95.19	64.50	20.09	7.39	0
13	0	0	-1.68	55.81	52.14	20.09	7.39	0
14	0	0	1.68	75.97	62.22	20.09	7.39	0
15	0	0	0	80.00	60.00	20.09	7.39	0
16	0	0	0	80.00	60.00	20.09	7.39	0
17	0	0	0	80.00	60.00	20.09	7.39	0
18	0	0	0	80.00	60.00	20.09	7.39	0
19	0	0	0	80.00	60.00	20.09	7.39	0
20	0	0	0	80.00	60.00	20.09	7.39	0

Table A.2 Data generated at experimental design points (scenario 1)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	73.06	67.54	75.56	76.29	69.86	55.24	55.23	51.90	52.89	52.47
2	48.16	52.25	46.36	58.78	48.39	64.31	66.90	64.16	63.74	61.74
3	88.32	81.01	90.20	94.28	83.90	56.33	57.41	49.67	50.08	55.55
4	67.21	72.09	72.66	72.19	74.78	63.82	65.24	58.73	61.95	61.57
5	63.81	72.15	66.27	77.34	67.39	59.44	58.60	55.49	52.10	57.84
6	88.47	95.75	95.28	100.58	95.65	64.25	67.03	63.26	65.95	65.87
7	67.00	65.58	71.91	58.60	68.92	66.43	65.99	65.57	64.11	65.84
8	99.55	95.85	95.31	95.67	90.39	67.36	68.32	68.86	71.92	67.05
9	75.47	76.26	76.89	68.23	73.63	56.75	53.36	54.09	59.04	55.74
10	77.78	76.43	73.19	73.53	78.02	66.96	71.67	71.09	67.31	68.82
11	76.42	71.88	86.17	79.42	83.21	61.78	61.20	58.41	58.57	60.12
12	89.87	90.45	101.79	95.44	89.73	64.39	61.44	60.83	63.79	67.09
13	56.38	58.75	50.57	53.74	54.63	48.84	48.55	54.67	52.17	50.38
14	79.58	77.01	71.53	81.97	77.27	66.24	65.31	60.36	58.71	62.02
15	78.52	76.22	82.23	86.67	77.55	57.70	59.33	61.80	57.68	56.73
16	79.46	79.71	82.17	77.33	79.33	58.82	59.78	64.17	58.35	56.34
17	82.10	75.95	80.16	77.19	82.40	61.50	59.45	54.42	60.36	64.33
18	84.56	72.92	79.65	76.95	75.41	56.64	60.79	58.83	60.15	59.00
19	77.92	81.66	83.26	89.47	73.92	57.22	62.82	58.94	56.25	60.86
20	86.96	83.17	88.77	82.26	88.36	59.08	56.90	59.43	63.24	56.97

Table A.3 Data generated at experimental design points (scenario 2)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	73.06	67.54	75.56	76.29	69.86	80.34	80.33	74.83	76.47	75.78	74.16	78.25	72.36
2	44.47	51.75	51.28	56.58	51.65	46.12	50.70	44.48	48.91	48.78	49.00	47.58	53.91
3	81.68	77.13	91.42	84.68	88.47	88.05	87.10	82.50	82.76	85.32	81.69	82.27	93.60
4	68.46	68.71	71.17	66.33	68.33	67.05	68.64	75.88	66.28	62.96	71.10	64.95	69.16
5	73.85	68.30	73.47	66.07	71.39	62.02	68.79	73.07	69.56	76.54	68.17	60.58	65.48
6	97.44	93.98	94.17	98.44	91.77	92.40	87.31	85.54	89.85	94.26	90.57	87.02	97.81
7	62.98	67.61	66.38	61.79	72.31	66.93	69.40	63.79	64.06	68.41	67.48	75.28	65.77
8	98.98	102.74	94.77	91.99	100.62	97.18	93.61	96.60	88.00	101.86	92.60	93.91	103.00
9	72.35	73.93	78.83	73.48	70.25	80.00	76.37	73.71	75.69	70.40	76.51	73.88	75.48
10	75.51	76.79	73.79	72.88	78.31	74.15	77.06	71.74	75.38	79.37	72.04	76.66	74.98
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	60.93	62.76	62.01	52.41	57.79	59.89	50.99	56.71	59.23	50.03	51.54	59.30	55.78
14	75.58	77.43	74.47	74.52	74.25	71.70	77.01	81.50	73.38	73.72	79.21	76.15	82.88
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table A.3 (cont’d) Data generated at at experimental design points (scenario 2)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	84.78	74.39	75.51	79.78	75.27	74.57	71.27	76.32	69.01	78.20	82.28	71.90
2	40.60	50.92	53.01	52.28	51.59	49.18	52.03	51.55	47.85	47.31	47.67	42.39
3	87.25	81.54	86.82	81.94	80.95	85.83	91.27	87.58	89.94	81.77	84.94	85.82
4	66.19	71.40	71.48	68.09	59.79	69.59	76.14	73.56	61.92	68.65	65.95	64.41
5	75.73	70.49	72.70	75.23	61.50	68.11	67.84	66.44	70.18	77.82	70.83	76.50
6	89.81	92.95	93.00	91.88	94.78	91.82	85.54	88.39	94.09	87.37	91.44	88.78
7	76.92	73.76	58.28	59.47	64.43	66.17	67.04	70.75	63.76	63.77	66.10	66.91
8	92.93	95.15	94.73	104.26	97.36	92.16	91.96	104.78	105.68	104.33	91.37	96.04
9	67.98	79.56	74.62	64.08	74.78	78.39	75.54	78.86	78.59	68.60	62.34	80.69
10	75.70	74.43	66.72	75.39	82.28	78.96	74.35	73.07	77.15	74.32	73.67	76.28
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	58.16	61.92	57.97	52.28	59.18	55.06	52.15	65.19	56.17	51.61	58.66	63.35
14	68.34	71.34	72.55	85.72	77.90	73.98	76.10	74.55	80.35	76.05	79.63	79.12
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table A.3 (cont'd) Data generated at experimental design points (scenario 2)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	54.33	55.41	47.67	48.08	53.55	50.91	53.88	54.22	53.94	55.51	53.82	55.24	48.73
2	63.36	64.32	64.86	67.92	63.05	65.69	66.17	66.56	61.30	64.58	64.65	61.26	61.98
3	50.70	50.41	56.53	54.03	52.25	56.19	54.63	51.31	57.64	54.79	58.02	57.09	52.14
4	58.64	62.79	60.83	62.15	61.00	60.74	63.01	63.98	67.74	58.31	59.22	64.82	60.94
5	56.11	58.02	55.87	59.60	57.32	59.31	59.82	57.79	60.42	64.28	59.43	57.97	60.48
6	62.81	63.22	64.91	66.47	65.68	68.89	65.33	61.87	66.03	66.19	66.86	67.36	69.47
7	64.76	66.88	65.69	59.24	65.90	66.21	65.73	67.56	64.89	62.17	63.59	57.34	65.29
8	67.46	68.84	66.44	65.34	66.79	70.94	74.45	68.62	67.28	69.91	66.67	73.06	71.01
9	57.16	56.16	55.00	51.93	56.70	52.37	53.82	55.54	58.16	57.12	52.45	60.13	56.19
10	72.95	62.69	71.13	66.80	72.11	62.95	68.93	69.70	68.39	68.99	65.43	66.48	67.33
11	62.99	62.65	63.87	64.57	61.26	60.29	61.76	63.85	64.45	59.67	63.62	60.67	60.23
12	65.15	63.55	66.93	68.79	61.49	64.43	61.48	66.54	65.86	63.10	62.98	62.45	67.02
13	53.75	54.29	52.42	51.71	54.50	51.61	52.34	50.71	50.27	51.41	48.91	52.81	52.42
14	61.59	61.91	62.57	60.04	61.57	61.97	59.44	64.77	59.14	60.29	59.04	65.11	60.37
15	56.66	59.25	59.56	57.05	54.69	57.53	59.98	55.32	63.43	58.37	54.39	60.30	64.04
16	62.61	55.50	57.31	61.86	57.35	58.35	61.87	60.05	62.89	56.35	61.30	55.56	56.08
17	63.01	60.67	60.45	61.10	63.31	63.94	57.21	60.56	61.60	59.28	66.78	62.33	57.69
18	60.62	56.11	59.59	58.63	55.30	58.87	58.33	61.96	60.92	62.40	60.77	59.60	59.76
19	61.25	61.71	61.03	57.25	59.06	61.20	55.68	58.09	57.07	62.72	64.70	61.93	57.97
20	59.02	61.50	55.77	59.44	58.84	61.34	57.63	60.22	58.58	56.16	58.96	58.76	59.21

Table A.3 (cont'd) Data generated at at experimental design points (scenario 2)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	51.95	51.57	47.64	52.70	49.13	55.85	49.81	53.44	52.60	49.49	46.10	51.84
2	66.94	63.64	65.06	64.24	62.27	62.48	65.21	61.42	66.12	65.55	61.77	63.28
3	50.49	53.80	53.10	51.71	55.35	58.05	52.51	51.70	53.33	55.80	51.68	50.73
4	58.25	62.86	66.22	63.92	67.32	63.37	67.07	61.08	58.90	61.43	65.24	58.97
5	58.15	54.99	59.32	57.99	57.25	61.47	63.07	56.58	58.28	55.80	59.85	51.57
6	64.51	66.71	65.96	64.42	71.81	65.30	62.17	70.81	66.88	62.96	67.69	69.45
7	64.32	62.39	62.22	61.06	63.87	65.03	63.10	62.64	63.90	63.52	61.40	67.51
8	64.66	66.18	71.65	69.05	69.07	63.36	68.62	69.86	66.27	65.27	67.50	65.13
9	61.19	52.82	53.97	54.02	55.81	53.45	53.48	49.64	53.82	56.80	55.60	55.65
10	70.54	67.95	73.72	69.92	64.48	68.31	67.77	69.82	68.94	68.78	67.55	69.37
11	62.61	63.68	59.59	57.07	61.01	62.65	61.37	65.43	60.24	63.30	59.01	57.71
12	63.83	64.10	61.08	65.35	71.82	65.29	60.63	65.17	60.60	64.91	59.90	66.46
13	52.03	46.03	50.75	52.82	53.14	52.62	52.04	47.78	53.06	51.78	53.46	53.77
14	57.53	64.43	66.14	64.05	62.59	59.88	60.17	65.56	65.35	60.56	64.41	62.81
15	60.14	60.44	59.93	60.47	62.40	60.50	62.05	61.38	60.36	60.76	57.33	57.43
16	60.80	59.62	56.93	59.20	58.42	57.56	60.68	55.95	60.85	54.50	61.44	60.93
17	62.21	61.90	62.07	55.34	64.18	55.62	63.02	56.98	61.05	62.62	62.22	60.10
18	60.79	63.17	62.19	56.31	60.33	59.40	61.55	59.18	63.08	59.51	56.01	63.79
19	60.62	59.39	57.68	60.94	60.30	56.92	58.14	59.24	61.78	56.61	58.38	58.69
20	59.18	55.68	62.97	63.60	59.66	58.00	60.58	58.91	60.18	55.22	64.59	60.89

Table A.4 Estimated model parameters (scenario 1)

$\hat{\boldsymbol{\beta}}$	**Real**		**OLS (Variance Known)**		**OLS**		**WLS**		**SUR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.72	59.23	80.72	59.23	80.57	59.08	80.72	59.23
$\hat{\beta}_1$	1.00	4.00	1.48	3.90	1.48	3.90	1.11	3.78	1.48	3.90
$\hat{\beta}_2$	4.00	1.00	4.17	1.21	4.17	1.21	4.28	1.20	4.17	1.21
$\hat{\beta}_3$	6.00	3.00	5.99	3.08	5.99	3.08	6.16	3.14	5.99	3.08
$\hat{\beta}_{11}$	-2.00	1.00	-1.93	1.33	-1.93	1.33	-2.04	1.40	-1.93	1.33
$\hat{\beta}_{22}$	3.00	1.00	2.14	1.07	2.14	1.07	2.47	1.13	2.14	1.07
$\hat{\beta}_{33}$	-5.00	-1.00	-5.05	-0.72	-5.05	-0.72	-5.04	-0.56	-5.05	-0.72
$\hat{\beta}_{12}$	2.00	-1.00	1.14	-0.95	1.14	-0.95	1.53	-1.01	1.14	-0.95
$\hat{\beta}_{13}$	12.00	-1.00	11.52	-0.92	11.52	-0.92	11.28	-0.93	11.52	-0.92
$\hat{\beta}_{23}$	-4.00	1.00	-4.86	1.75	-4.86	1.75	-5.20	1.88	-4.86	1.75

Table A.5 Prediction at the center point (scenario 1)

Real		**OLS (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.72	59.23	80.72	59.23	80.57	59.08	80.72	59.23

Table A.6 Prediction at the corner point (scenario 1)

Real		**OLS (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	95.31	68.97	95.31	68.97	95.13	69.11	95.31	68.97

Table A.7 Estimated model parameters (scenario 2)

	Real		**OLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.21	59.68	80.21	59.68	80.16	59.64	80.21	59.68
$\hat{\beta}_1$	1.00	4.00	0.76	4.04	0.76	4.04	0.74	4.05	0.76	4.04
$\hat{\beta}_2$	4.00	1.00	3.49	0.87	3.49	0.87	3.48	0.87	3.49	0.87
$\hat{\beta}_3$	6.00	3.00	5.80	3.04	5.80	3.04	5.82	3.05	5.80	3.04
$\hat{\beta}_{11}$	-2.00	1.00	-2.07	0.84	-2.07	0.84	-2.12	0.86	-2.07	0.84
$\hat{\beta}_{22}$	3.00	1.00	2.46	1.28	2.46	1.28	2.47	1.30	2.46	1.28
$\hat{\beta}_{33}$	-5.00	-1.00	-4.88	-0.88	-4.88	-0.88	-4.85	-0.89	-4.88	-0.88
$\hat{\beta}_{12}$	2.00	-1.00	2.24	-0.89	2.24	-0.89	2.26	-0.92	2.24	-0.89
$\hat{\beta}_{13}$	12.00	-1.00	11.90	-1.10	11.90	-1.10	11.84	-1.11	11.90	-1.10
$\hat{\beta}_{23}$	-4.00	1.00	-3.32	0.92	-3.32	0.92	-3.39	0.93	-3.32	0.92

Table A.8 Prediction at the center point (scenario 2)

Real		**OLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.21	59.68	80.21	59.68	80.16	59.64	80.21	59.68

Table A.9 Prediction at the corner point (scenario 2)

Real		**OLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	96.58	67.80	96.58	67.80	96.41	67.78	96.58	67.80

APPENDIX B

GENERATED DATA AND MODEL PARAMETER ESTIMATES UNDER SCENARIOS 3-4: WLS CASE

Table B.1 True mean, variance and covariance values at experimental design points (scenarios 3&4)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	52.00	0.37	0.37	0.00
2	1	-1	-1	49.00	64.00	0.37	0.37	0.00
3	-1	1	-1	87.00	54.00	0.37	0.37	0.00
4	1	1	-1	69.00	62.00	0.37	0.37	0.00
5	-1	-1	1	71.00	58.00	0.37	0.37	0.00
6	1	-1	1	93.00	66.00	0.37	0.37	0.00
7	-1	1	1	67.00	64.00	0.37	0.37	0.00
8	1	1	1	97.00	68.00	0.37	0.37	0.00
9	-1.68	0	0	72.68	56.10	1.19	0.03	0.00
10	1.68	0	0	76.04	69.54	1.19	0.03	0.00
11	0	-1.68	0	81.75	61.14	20.09	7.39	0.00
12	0	1.68	0	95.19	64.50	20.09	7.39	0.00
13	0	0	-1.68	55.81	52.14	0.00	0.44	0.00
14	0	0	1.68	75.97	62.22	0.00	0.44	0.00
15	0	0	0	80.00	60.00	20.09	7.39	0.00
16	0	0	0	80.00	60.00	20.09	7.39	0.00
17	0	0	0	80.00	60.00	20.09	7.39	0.00
18	0	0	0	80.00	60.00	20.09	7.39	0.00
19	0	0	0	80.00	60.00	20.09	7.39	0.00
20	0	0	0	80.00	60.00	20.09	7.39	0.00

Table B.2 Data generated at experimental design points (scenario 3)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	74.74	73.99	75.08	75.17	74.30	52.72	52.72	51.98	52.20	52.11
2	48.89	49.44	48.64	50.32	48.92	64.07	64.65	64.04	63.94	63.50
3	87.18	86.19	87.43	87.98	86.58	54.52	54.76	53.03	53.13	54.35
4	68.76	69.42	69.49	69.43	69.78	62.41	62.72	61.27	61.99	61.90
5	70.03	71.16	70.36	71.86	70.51	58.32	58.13	57.44	56.68	57.96
6	92.39	93.37	93.31	94.03	93.36	65.61	66.23	65.39	65.99	65.97
7	67.00	66.81	67.66	65.86	67.26	64.54	64.44	64.35	64.02	64.41
8	97.35	96.84	96.77	96.82	96.11	67.86	68.07	68.19	68.88	67.79
9	73.36	73.55	73.70	71.59	72.91	56.14	55.94	55.98	56.28	56.08
10	76.46	76.13	75.34	75.42	76.52	69.39	69.67	69.63	69.41	69.50
11	76.42	71.88	86.17	79.42	83.21	61.78	61.20	58.41	58.57	60.12
12	89.87	90.45	101.79	95.44	89.73	64.39	61.44	60.83	63.79	67.09
13	55.82	55.85	55.73	55.78	55.79	51.33	51.26	52.75	52.15	51.71
14	76.02	75.98	75.90	76.06	75.99	63.20	62.97	61.76	61.36	62.17
15	78.52	76.22	82.23	86.67	77.55	57.70	59.33	61.80	57.68	56.73
16	79.46	79.71	82.17	77.33	79.33	58.82	59.78	64.17	58.35	56.34
17	82.10	75.95	80.16	77.19	82.40	61.50	59.45	54.42	60.36	64.33
18	84.56	72.92	79.65	76.95	75.41	56.64	60.79	58.83	60.15	59.00
19	77.92	81.66	83.26	89.47	73.92	57.22	62.82	58.94	56.25	60.86
20	86.96	83.17	88.77	82.26	88.36	59.08	56.90	59.43	63.24	56.97

Table B.3 Data generated at experimental design points (scenario 4)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	74.74	73.99	75.08	75.17	74.30	75.72	75.72	74.98	75.20	75.11	74.89	75.44	74.64
2	48.39	49.37	49.31	50.03	49.36	48.61	49.23	48.39	48.99	48.97	49.00	48.81	49.66
3	86.28	85.66	87.60	86.69	87.20	87.14	87.01	86.39	86.43	86.77	86.28	86.36	87.89
4	68.93	68.96	69.29	68.64	68.91	68.74	68.95	69.93	68.63	68.18	69.28	68.45	69.02
5	71.39	70.64	71.33	70.33	71.05	69.78	70.70	71.28	70.81	71.75	70.62	69.59	70.25
6	93.60	93.13	93.16	93.74	92.83	92.92	92.23	91.99	92.57	93.17	92.67	92.19	93.65
7	66.46	67.08	66.92	66.29	67.72	66.99	67.33	66.57	66.60	67.19	67.06	68.12	66.83
8	97.27	97.78	96.70	96.32	97.49	97.02	96.54	96.95	95.78	97.66	96.40	96.58	97.81
9	72.60	72.98	74.18	72.87	72.08	74.46	73.58	72.93	73.41	72.12	73.61	72.97	73.36
10	75.91	76.22	75.49	75.26	76.59	75.58	76.29	74.99	75.88	76.85	75.06	76.19	75.78
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	55.88	55.91	55.90	55.76	55.84	55.87	55.74	55.82	55.86	55.72	55.75	55.86	55.81
14	75.96	75.99	75.95	75.95	75.94	75.91	75.98	76.05	75.93	75.94	76.01	75.97	76.07
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table B.3 (cont'd) Data generated at experimental design points (scenario 4)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	76.32	74.92	75.07	75.65	75.04	74.94	74.50	75.18	74.19	75.43	75.98	74.58
2	47.86	49.26	49.54	49.44	49.35	49.02	49.41	49.35	48.84	48.77	48.82	48.11
3	87.03	86.26	86.97	86.32	86.18	86.84	87.58	87.08	87.40	86.29	86.72	86.84
4	68.62	69.32	69.34	68.88	67.75	69.08	69.97	69.62	68.04	68.95	68.59	68.38
5	71.64	70.93	71.23	71.57	69.71	70.61	70.57	70.38	70.89	71.92	70.98	71.74
6	92.57	92.99	93.00	92.85	93.24	92.84	91.99	92.38	93.15	92.24	92.79	92.43
7	68.34	67.91	65.82	65.98	66.65	66.89	67.01	67.51	66.56	66.56	66.88	66.99
8	96.45	96.75	96.69	97.98	97.05	96.34	96.32	98.05	98.18	97.99	96.24	96.87
9	71.53	74.35	73.15	70.58	73.19	74.07	73.37	74.18	74.12	71.68	70.16	74.63
10	75.95	75.64	73.76	75.88	77.56	76.75	75.62	75.31	76.31	75.62	75.46	76.10
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	55.84	55.90	55.84	55.76	55.86	55.80	55.75	55.94	55.81	55.75	55.85	55.92
14	75.86	75.90	75.92	76.11	76.00	75.94	75.97	75.95	76.03	75.97	76.02	76.01
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table B.3 (cont'd) Data generated at experimental design points (scenario 4)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	52.52	52.76	51.03	51.13	52.35	51.76	52.42	52.49	52.43	52.78	52.41	52.72	51.27
2	63.86	64.07	64.19	64.88	63.79	64.38	64.48	64.57	63.40	64.13	64.14	63.39	63.55
3	53.26	53.20	54.56	54.01	53.61	54.49	54.14	53.40	54.81	54.18	54.90	54.69	53.59
4	61.25	62.18	61.74	62.03	61.78	61.72	62.22	62.44	63.28	61.18	61.38	62.63	61.76
5	57.58	58.00	57.53	58.36	57.85	58.29	58.41	57.95	58.54	59.40	58.32	57.99	58.55
6	65.29	65.38	65.76	66.11	65.93	66.65	65.85	65.08	66.01	66.04	66.19	66.30	66.78
7	64.17	64.64	64.38	62.94	64.42	64.49	64.39	64.79	64.20	63.59	63.91	62.51	64.29
8	67.88	68.19	67.65	67.41	67.73	68.66	69.44	68.14	67.84	68.43	67.70	69.13	68.67
9	56.17	56.11	56.04	55.85	56.14	55.88	55.97	56.07	56.22	56.16	55.88	56.34	56.11
10	69.75	69.14	69.64	69.38	69.70	69.15	69.51	69.55	69.47	69.51	69.30	69.36	69.41
11	62.99	62.65	63.87	64.57	61.26	60.29	61.76	63.85	64.45	59.67	63.62	60.67	60.23
12	65.15	63.55	66.93	68.79	61.49	64.43	61.48	66.54	65.86	63.10	62.98	62.45	67.02
13	52.53	52.66	52.21	52.03	52.71	52.01	52.19	51.79	51.68	51.96	51.35	52.30	52.21
14	62.06	62.14	62.30	61.69	62.06	62.16	61.54	62.84	61.47	61.75	61.44	62.92	61.77
15	56.66	59.25	59.56	57.05	54.69	57.53	59.98	55.32	63.43	58.37	54.39	60.30	64.04
16	62.61	55.50	57.31	61.86	57.35	58.35	61.87	60.05	62.89	56.35	61.30	55.56	56.08
17	63.01	60.67	60.45	61.10	63.31	63.94	57.21	60.56	61.60	59.28	66.78	62.33	57.69
18	60.62	56.11	59.59	58.63	55.30	58.87	58.33	61.96	60.92	62.40	60.77	59.60	59.76
19	61.25	61.71	61.03	57.25	59.06	61.20	55.68	58.09	57.07	62.72	64.70	61.93	57.97
20	59.02	61.50	55.77	59.44	58.84	61.34	57.63	60.22	58.58	56.16	58.96	58.76	59.21

Table B.3 (cont'd) Data generated at experimental design points (scenario 4)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	51.99	51.90	51.03	52.16	51.36	52.86	51.51	52.32	52.13	51.44	50.68	51.96
2	64.66	63.92	64.24	64.05	63.61	63.66	64.27	63.42	64.47	64.35	63.50	63.84
3	53.22	53.96	53.80	53.49	54.30	54.90	53.67	53.49	53.85	54.40	53.48	53.27
4	61.16	62.19	62.94	62.43	63.19	62.31	63.13	61.79	61.31	61.87	62.72	61.32
5	58.03	57.33	58.29	58.00	57.83	58.77	59.13	57.68	58.06	57.51	58.41	56.57
6	65.67	66.16	65.99	65.65	67.30	65.84	65.15	67.07	66.20	65.32	66.38	66.77
7	64.07	63.64	63.60	63.34	63.97	64.23	63.80	63.70	63.98	63.89	63.42	64.78
8	67.26	67.59	68.81	68.24	68.24	66.96	68.14	68.42	67.61	67.39	67.89	67.36
9	56.40	55.91	55.98	55.98	56.09	55.94	55.95	55.72	55.97	56.14	56.07	56.08
10	69.60	69.45	69.79	69.57	69.24	69.47	69.44	69.56	69.51	69.50	69.42	69.53
11	62.61	63.68	59.59	57.07	61.01	62.65	61.37	65.43	60.24	63.30	59.01	57.71
12	63.83	64.10	61.08	65.35	71.82	65.29	60.63	65.17	60.60	64.91	59.90	66.46
13	52.11	50.65	51.80	52.30	52.38	52.26	52.11	51.07	52.36	52.05	52.46	52.53
14	61.07	62.76	63.17	62.66	62.31	61.65	61.72	63.03	62.98	61.81	62.75	62.36
15	60.14	60.44	59.93	60.47	62.40	60.50	62.05	61.38	60.36	60.76	57.33	57.43
16	60.80	59.62	56.93	59.20	58.42	57.56	60.68	55.95	60.85	54.50	61.44	60.93
17	62.21	61.90	62.07	55.34	64.18	55.62	63.02	56.98	61.05	62.62	62.22	60.10
18	60.79	63.17	62.19	56.31	60.33	59.40	61.55	59.18	63.08	59.51	56.01	63.79
19	60.62	59.39	57.68	60.94	60.30	56.92	58.14	59.24	61.78	56.61	58.38	58.69
20	59.18	55.68	62.97	63.60	59.66	58.00	60.58	58.91	60.18	55.22	64.59	60.89

Table B.4 Estimated model parameters (scenario 3)

$\hat{\boldsymbol{\beta}}$	**Real**		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.63	59.20	80.72	59.25	80.55	59.02	80.72	59.25
$\hat{\beta}_1$	1.00	4.00	1.11	4.00	1.04	3.98	1.06	3.99	1.04	3.98
$\hat{\beta}_2$	4.00	1.00	4.02	1.07	4.09	1.06	4.03	1.07	4.09	1.06
$\hat{\beta}_3$	6.00	3.00	6.01	3.01	5.96	3.02	6.01	3.02	5.96	3.02
$\hat{\beta}_{11}$	-2.00	1.00	-2.13	1.28	-2.06	1.35	-2.18	1.34	-2.06	1.35
$\hat{\beta}_{22}$	3.00	1.00	2.72	1.28	2.18	0.98	2.86	1.34	2.18	0.98
$\hat{\beta}_{33}$	-5.00	-1.00	-5.23	-0.73	-5.11	-0.69	-5.20	-0.66	-5.11	-0.69
$\hat{\beta}_{12}$	2.00	-1.00	1.88	-0.99	1.88	-0.99	1.92	-1.00	1.88	-0.99
$\hat{\beta}_{13}$	12.00	-1.00	11.93	-0.98	11.93	-0.98	11.91	-0.98	11.93	-0.98
$\hat{\beta}_{23}$	-4.00	1.00	-4.12	1.17	-4.12	1.17	-4.15	1.20	-4.12	1.17

Table B.5 Prediction at the center point (scenario 3)

Real		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.63	59.20	80.72	59.25	80.55	59.02	80.72	59.25

Table B.6 Prediction at the corner point (scenario 3)

Real		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	96.83	68.30	96.52	68.14	96.80	68.33	96.52	68.14

Table B.7 Estimated model parameters (scenario 4)

	Real		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.15	59.70	80.18	59.70	80.09	59.67	80.18	59.70
$\hat{\beta}_1$	1.00	4.00	0.98	4.00	0.94	4.01	0.97	4.00	0.94	4.01
$\hat{\beta}_2$	4.00	1.00	3.97	0.98	3.56	0.90	3.96	0.97	3.56	0.90
$\hat{\beta}_3$	6.00	3.00	6.00	3.01	5.99	3.01	6.00	3.01	5.99	3.01
$\hat{\beta}_{11}$	-2.00	1.00	-2.01	1.08	-1.98	1.08	-2.02	1.10	-1.98	1.08
$\hat{\beta}_{22}$	3.00	1.00	2.83	1.15	2.64	1.18	2.89	1.17	2.64	1.18
$\hat{\beta}_{33}$	-5.00	-1.00	-5.05	-0.92	-5.01	-0.92	-5.03	-0.90	-5.01	-0.92
$\hat{\beta}_{12}$	2.00	-1.00	2.03	-0.97	2.03	-0.97	2.03	-0.97	2.03	-0.97
$\hat{\beta}_{13}$	12.00	-1.00	11.99	-1.02	11.99	-1.02	11.98	-1.02	11.99	-1.02
$\hat{\beta}_{23}$	-4.00	1.00	-3.91	0.98	-3.91	0.98	-3.91	0.98	-3.91	0.98

Table B.8 Prediction at the center point (scenario 4)

Real		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.15	59.70	80.18	59.70	80.09	59.67	80.18	59.70

Table B.9 Prediction at the corner point (scenario 4)

Real		**WLS (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	96.97	68.00	96.42	67.94	96.95	68.00	96.42	67.94

APPENDIX C

GENERATED DATA AND MODEL PARAMETER ESTIMATES UNDER SCENARIOS 5-8: MVR CASE

Table C.1 True mean, variance and covariance values at experimental design points (scenarios 5&6)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	52.00	20.09	7.39	3.65
2	1	-1	-1	49.00	64.00	20.09	7.39	3.65
3	-1	1	-1	87.00	54.00	20.09	7.39	3.65
4	1	1	-1	69.00	62.00	20.09	7.39	3.65
5	-1	-1	1	71.00	58.00	20.09	7.39	3.65
6	1	-1	1	93.00	66.00	20.09	7.39	3.65
7	-1	1	1	67.00	64.00	20.09	7.39	3.65
8	1	1	1	97.00	68.00	20.09	7.39	3.65
9	-1.68	0	0	72.68	56.10	20.09	7.39	3.65
10	1.68	0	0	76.04	69.54	20.09	7.39	3.65
11	0	-1.68	0	81.75	61.14	20.09	7.39	3.65
12	0	1.68	0	95.19	64.50	20.09	7.39	3.65
13	0	0	-1.68	55.81	52.14	20.09	7.39	3.65
14	0	0	1.68	75.97	62.22	20.09	7.39	3.65
15	0	0	0	80.00	60.00	20.09	7.39	3.65
16	0	0	0	80.00	60.00	20.09	7.39	3.65
17	0	0	0	80.00	60.00	20.09	7.39	3.65
18	0	0	0	80.00	60.00	20.09	7.39	3.65
19	0	0	0	80.00	60.00	20.09	7.39	3.65
20	0	0	0	80.00	60.00	20.09	7.39	3.65

Table C.2 True mean, variance and covariance values at experimental design points (scenarios 7&8)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	52.00	20.09	7.39	10.96
2	1	-1	-1	49.00	64.00	20.09	7.39	10.96
3	-1	1	-1	87.00	54.00	20.09	7.39	10.96
4	1	1	-1	69.00	62.00	20.09	7.39	10.96
5	-1	-1	1	71.00	58.00	20.09	7.39	10.96
6	1	-1	1	93.00	66.00	20.09	7.39	10.96
7	-1	1	1	67.00	64.00	20.09	7.39	10.96
8	1	1	1	97.00	68.00	20.09	7.39	10.96
9	-1.68	0	0	72.68	56.10	20.09	7.39	10.96
10	1.68	0	0	76.04	69.54	20.09	7.39	10.96
11	0	-1.68	0	81.75	61.14	20.09	7.39	10.96
12	0	1.68	0	95.19	64.50	20.09	7.39	10.96
13	0	0	-1.68	55.81	52.14	20.09	7.39	10.96
14	0	0	1.68	75.97	62.22	20.09	7.39	10.96
15	0	0	0	80.00	60.00	20.09	7.39	10.96
16	0	0	0	80.00	60.00	20.09	7.39	10.96
17	0	0	0	80.00	60.00	20.09	7.39	10.96
18	0	0	0	80.00	60.00	20.09	7.39	10.96
19	0	0	0	80.00	60.00	20.09	7.39	10.96
20	0	0	0	80.00	60.00	20.09	7.39	10.96

Table C.3 Data generated at experimental design points (scenario 5)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	73.06	67.54	75.56	76.29	69.86	54.74	53.73	52.00	53.08	51.52
2	48.16	52.25	46.36	58.78	48.39	64.14	67.36	63.67	65.53	61.73
3	88.32	81.01	90.20	94.28	83.90	56.46	56.16	50.45	51.59	54.92
4	67.21	72.09	72.66	72.19	74.78	63.41	65.65	59.55	62.53	62.65
5	63.81	72.15	66.27	77.34	67.39	58.06	58.78	54.75	53.53	57.19
6	88.47	95.75	95.28	100.58	95.65	63.51	67.49	63.80	67.33	66.36
7	67.00	65.58	71.91	58.60	68.92	66.32	65.64	66.39	62.58	66.10
8	99.55	95.85	95.31	95.67	90.39	67.86	68.10	68.51	71.50	65.89
9	75.47	76.26	76.89	68.23	73.63	57.23	54.14	54.95	58.10	55.93
10	77.78	76.43	73.19	73.53	78.02	67.40	71.64	70.50	66.96	69.22
11	76.42	71.88	86.17	79.42	83.21	60.78	59.40	59.34	58.26	60.44
12	89.87	90.45	101.79	95.44	89.73	63.43	60.72	62.20	63.87	65.98
13	56.38	58.75	50.57	53.74	54.63	49.10	49.25	53.60	51.79	50.25
14	79.58	77.01	71.53	81.97	77.27	66.71	65.36	59.64	59.96	62.26
15	78.52	76.22	82.23	86.67	77.55	57.53	58.67	62.13	59.00	56.44
16	79.46	79.71	82.17	77.33	79.33	58.77	59.74	64.38	57.94	56.38
17	82.10	75.95	80.16	77.19	82.40	61.82	58.73	54.70	59.83	64.57
18	84.56	72.92	79.65	76.95	75.41	57.63	59.46	58.82	59.59	58.21
19	77.92	81.66	83.26	89.47	73.92	56.97	62.99	59.58	58.14	59.71
20	86.96	83.17	88.77	82.26	88.36	60.39	57.62	61.05	63.50	58.63

Table C.4 Data generated at experimental design points (scenario 6)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	73.06	67.54	75.56	76.29	69.86	80.34	80.33	74.83	76.47	75.78	74.16	78.25	72.36
2	44.47	51.75	51.28	56.58	51.65	46.12	50.70	44.48	48.91	48.78	49.00	47.58	53.91
3	81.68	77.13	91.42	84.68	88.47	88.05	87.10	82.50	82.76	85.32	81.69	82.27	93.60
4	68.46	68.71	71.17	66.33	68.33	67.05	68.64	75.88	66.28	62.96	71.10	64.95	69.16
5	73.85	68.30	73.47	66.07	71.39	62.02	68.79	73.07	69.56	76.54	68.17	60.58	65.48
6	97.44	93.98	94.17	98.44	91.77	92.40	87.31	85.54	89.85	94.26	90.57	87.02	97.81
7	62.98	67.61	66.38	61.79	72.31	66.93	69.40	63.79	64.06	68.41	67.48	75.28	65.77
8	98.98	102.74	94.77	91.99	100.62	97.18	93.61	96.60	88.00	101.86	92.60	93.91	103.00
9	72.35	73.93	78.83	73.48	70.25	80.00	76.37	73.71	75.69	70.40	76.51	73.88	75.48
10	75.51	76.79	73.79	72.88	78.31	74.15	77.06	71.74	75.38	79.37	72.04	76.66	74.98
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	60.93	62.76	62.01	52.41	57.79	59.89	50.99	56.71	59.23	50.03	51.54	59.30	55.78
14	75.58	77.43	74.47	74.52	74.25	71.70	77.01	81.50	73.38	73.72	79.21	76.15	82.88
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table C.4 (cont'd) Data generated at experimental design points (scenario 6)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	84.78	74.39	75.51	79.78	75.27	74.57	71.27	76.32	69.01	78.20	82.28	71.90
2	40.60	50.92	53.01	52.28	51.59	49.18	52.03	51.55	47.85	47.31	47.67	42.39
3	87.25	81.54	86.82	81.94	80.95	85.83	91.27	87.58	89.94	81.77	84.94	85.82
4	66.19	71.40	71.48	68.09	59.79	69.59	76.14	73.56	61.92	68.65	65.95	64.41
5	75.73	70.49	72.70	75.23	61.50	68.11	67.84	66.44	70.18	77.82	70.83	76.50
6	89.81	92.95	93.00	91.88	94.78	91.82	85.54	88.39	94.09	87.37	91.44	88.78
7	76.92	73.76	58.28	59.47	64.43	66.17	67.04	70.75	63.76	63.77	66.10	66.91
8	92.93	95.15	94.73	104.26	97.36	92.16	91.96	104.78	105.68	104.33	91.37	96.04
9	67.98	79.56	74.62	64.08	74.78	78.39	75.54	78.86	78.59	68.60	62.34	80.69
10	75.70	74.43	66.72	75.39	82.28	78.96	74.35	73.07	77.15	74.32	73.67	76.28
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	58.16	61.92	57.97	52.28	59.18	55.06	52.15	65.19	56.17	51.61	58.66	63.35
14	68.34	71.34	72.55	85.72	77.90	73.98	76.10	74.55	80.35	76.05	79.63	79.12
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table C.4 (cont'd) Data generated at experimental design points (scenario 6)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	53.87	53.89	47.97	48.50	52.55	51.93	54.76	54.08	54.11	55.49	53.58	55.68	48.40
2	62.57	64.81	65.23	69.12	63.57	65.09	66.38	65.62	61.41	64.51	64.62	61.13	62.97
3	49.89	48.78	57.22	53.61	52.59	56.28	54.62	50.61	56.70	54.45	56.87	56.09	53.43
4	58.70	62.70	61.28	61.66	60.92	60.44	62.90	65.14	66.98	57.38	59.73	63.95	61.02
5	56.71	57.53	56.42	58.63	57.42	57.61	59.33	58.17	60.04	65.00	58.85	56.07	59.36
6	63.76	63.53	65.17	67.44	65.47	68.65	64.33	60.71	65.45	66.41	66.38	66.21	70.19
7	63.99	66.85	65.50	58.51	66.77	66.09	66.09	66.81	64.31	62.51	63.70	59.16	65.00
8	67.84	69.84	66.11	64.55	67.50	70.84	73.54	68.52	65.67	70.70	65.94	72.27	71.96
9	57.06	56.38	56.17	52.27	56.23	53.87	54.60	55.75	58.61	56.66	53.31	60.16	56.70
10	72.70	63.15	70.65	66.35	72.41	62.91	69.15	68.91	68.32	69.62	64.89	66.74	67.24
11	61.73	63.08	62.66	63.87	61.14	60.53	61.67	65.14	65.62	60.25	63.58	60.04	59.90
12	65.67	62.46	65.76	68.10	60.41	64.89	61.40	65.39	65.07	62.36	62.99	60.58	66.34
13	54.61	55.45	53.54	51.11	54.76	52.38	51.46	50.94	50.98	50.39	48.28	53.42	52.40
14	61.55	62.19	62.28	59.88	61.29	61.21	59.75	65.66	58.81	59.97	59.77	65.01	61.71
15	56.51	58.61	59.82	55.71	53.65	59.29	59.93	57.67	63.08	58.58	55.40	60.14	63.43
16	62.47	56.00	56.70	62.44	57.56	60.65	62.12	58.99	63.07	56.93	60.83	55.95	55.77
17	63.49	60.07	60.98	60.18	63.89	62.02	57.57	59.93	60.90	59.44	66.20	63.01	57.71
18	59.84	56.20	58.96	57.33	54.78	59.40	58.86	61.53	60.93	62.66	60.90	59.83	61.46
19	61.55	62.09	60.42	58.05	57.28	62.04	55.88	56.86	56.20	62.77	64.66	61.02	57.69
20	59.87	62.87	57.13	60.21	59.16	61.34	56.52	59.87	58.63	56.52	58.18	58.27	59.70

Table C.4 (cont'd) Data generated at experimental design points (scenario 6)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	53.73	51.48	47.93	53.54	49.31	55.59	49.23	53.61	51.48	50.19	47.70	51.28
2	65.28	64.01	65.74	64.82	62.82	62.58	65.70	62.00	65.82	65.17	61.63	62.11
3	50.70	52.82	53.11	50.89	54.19	57.65	53.36	51.91	53.90	54.77	51.41	50.67
4	57.91	63.25	66.48	63.67	65.40	63.42	68.13	61.95	57.76	61.39	64.53	58.27
5	59.01	55.04	59.57	58.76	55.55	60.78	62.26	55.81	58.12	57.15	59.73	52.87
6	64.00	66.67	65.97	64.29	71.86	65.12	60.99	69.75	67.04	62.07	67.33	68.52
7	66.11	63.70	60.72	59.83	63.41	64.83	63.15	63.39	63.32	62.96	61.35	67.33
8	64.08	65.93	71.06	70.33	69.09	62.69	67.67	71.19	67.93	66.73	66.49	65.09
9	60.10	54.22	54.43	52.55	56.21	54.61	54.12	51.06	55.01	56.03	53.75	57.13
10	70.43	67.73	71.83	69.79	65.85	68.90	67.54	69.27	69.17	68.51	67.21	69.42
11	61.40	63.25	59.28	58.68	61.63	62.63	61.12	65.30	60.91	65.03	59.37	58.57
12	62.72	64.38	61.73	65.43	71.40	63.10	60.84	64.43	60.56	64.62	59.17	66.84
13	52.46	47.42	51.21	52.14	53.71	52.47	51.38	49.69	53.08	51.03	53.91	55.06
14	56.36	63.48	65.33	65.74	62.93	59.63	60.29	65.15	66.00	60.66	64.98	63.35
15	61.31	59.71	60.59	60.03	62.89	61.16	61.28	61.75	61.18	59.87	57.75	57.52
16	60.78	59.98	58.04	59.87	56.33	57.91	61.32	56.13	61.51	55.38	62.44	61.89
17	62.93	61.43	62.03	55.88	64.90	56.33	62.64	56.00	60.44	62.77	61.31	60.33
18	58.89	63.30	62.33	57.02	59.84	60.15	61.62	59.91	63.73	60.61	56.14	64.69
19	61.73	59.04	57.81	61.55	61.02	57.17	56.91	57.94	62.05	56.16	58.91	57.62
20	58.25	55.25	63.06	64.69	58.81	58.60	59.90	58.71	59.68	56.47	65.07	59.13

Table C.5 Data generated at experimental design points (scenario 7)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	73.06	67.54	75.56	76.29	69.86	52.35	49.33	52.26	53.09	49.40
2	48.16	52.25	46.36	58.78	48.39	63.68	67.04	62.63	69.23	62.68
3	88.32	81.01	90.20	94.28	83.90	55.74	52.22	53.86	56.26	52.98
4	67.21	72.09	72.66	72.19	74.78	61.81	65.10	62.57	63.72	64.97
5	63.81	72.15	66.27	77.34	67.39	54.70	58.89	54.32	58.89	55.96
6	88.47	95.75	95.28	100.58	95.65	62.76	67.95	66.05	70.12	67.39
7	67.00	65.58	71.91	58.60	68.92	65.06	64.09	67.36	59.46	65.85
8	99.55	95.85	95.31	95.67	90.39	69.11	67.51	67.45	68.99	63.98
9	75.47	76.26	76.89	68.23	73.63	57.91	56.86	57.53	54.96	56.47
10	77.78	76.43	73.19	73.53	78.02	69.37	70.68	68.66	67.20	70.31
11	76.42	71.88	86.17	79.42	83.21	58.51	55.78	62.37	58.75	61.50
12	89.87	90.45	101.79	95.44	89.73	61.55	60.58	66.51	64.33	62.65
13	56.38	58.75	50.57	53.74	54.63	51.01	52.18	50.38	51.02	50.73
14	79.58	77.01	71.53	81.97	77.27	65.94	64.13	58.99	63.96	62.84
15	78.52	76.22	82.23	86.67	77.55	58.19	57.64	62.00	62.63	57.24
16	79.46	79.71	82.17	77.33	79.33	59.19	59.75	63.01	57.82	58.04
17	82.10	75.95	80.16	77.19	82.40	61.80	57.55	57.65	58.62	63.20
18	84.56	72.92	79.65	76.95	75.41	61.03	56.48	59.30	58.40	57.06
19	77.92	81.66	83.26	89.47	73.92	57.65	62.14	61.32	63.53	57.05
20	86.96	83.17	88.77	82.26	88.36	63.40	60.38	64.54	62.64	63.24

Table C.6 Data generated at experimental design points (scenario 8)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	73.06	67.54	75.56	76.29	69.86	80.34	80.33	74.83	76.47	75.78	74.16	78.25	72.36
2	44.47	51.75	51.28	56.58	51.65	46.12	50.70	44.48	48.91	48.78	49.00	47.58	53.91
3	81.68	77.13	91.42	84.68	88.47	88.05	87.10	82.50	82.76	85.32	81.69	82.27	93.60
4	68.46	68.71	71.17	66.33	68.33	67.05	68.64	75.88	66.28	62.96	71.10	64.95	69.16
5	73.85	68.30	73.47	66.07	71.39	62.02	68.79	73.07	69.56	76.54	68.17	60.58	65.48
6	97.44	93.98	94.17	98.44	91.77	92.40	87.31	85.54	89.85	94.26	90.57	87.02	97.81
7	62.98	67.61	66.38	61.79	72.31	66.93	69.40	63.79	64.06	68.41	67.48	75.28	65.77
8	98.98	102.74	94.77	91.99	100.62	97.18	93.61	96.60	88.00	101.86	92.60	93.91	103.00
9	72.35	73.93	78.83	73.48	70.25	80.00	76.37	73.71	75.69	70.40	76.51	73.88	75.48
10	75.51	76.79	73.79	72.88	78.31	74.15	77.06	71.74	75.38	79.37	72.04	76.66	74.98
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	60.93	62.76	62.01	52.41	57.79	59.89	50.99	56.71	59.23	50.03	51.54	59.30	55.78
14	75.58	77.43	74.47	74.52	74.25	71.70	77.01	81.50	73.38	73.72	79.21	76.15	82.88
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table C.6 (cont'd) Data generated at experimental design points (scenario 8)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	84.78	74.39	75.51	79.78	75.27	74.57	71.27	76.32	69.01	78.20	82.28	71.90
2	40.60	50.92	53.01	52.28	51.59	49.18	52.03	51.55	47.85	47.31	47.67	42.39
3	87.25	81.54	86.82	81.94	80.95	85.83	91.27	87.58	89.94	81.77	84.94	85.82
4	66.19	71.40	71.48	68.09	59.79	69.59	76.14	73.56	61.92	68.65	65.95	64.41
5	75.73	70.49	72.70	75.23	61.50	68.11	67.84	66.44	70.18	77.82	70.83	76.50
6	89.81	92.95	93.00	91.88	94.78	91.82	85.54	88.39	94.09	87.37	91.44	88.78
7	76.92	73.76	58.28	59.47	64.43	66.17	67.04	70.75	63.76	63.77	66.10	66.91
8	92.93	95.15	94.73	104.26	97.36	92.16	91.96	104.78	105.68	104.33	91.37	96.04
9	67.98	79.56	74.62	64.08	74.78	78.39	75.54	78.86	78.59	68.60	62.34	80.69
10	75.70	74.43	66.72	75.39	82.28	78.96	74.35	73.07	77.15	74.32	73.67	76.28
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	58.16	61.92	57.97	52.28	59.18	55.06	52.15	65.19	56.17	51.61	58.66	63.35
14	68.34	71.34	72.55	85.72	77.90	73.98	76.10	74.55	80.35	76.05	79.63	79.12
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table C.6 (cont'd) Data generated at experimental design points (scenario 8)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	51.96	49.41	50.42	51.00	49.87	54.44	55.73	52.87	53.64	53.96	52.34	55.19	49.14
2	61.25	65.64	65.62	69.85	65.03	63.16	65.88	62.65	62.78	64.13	64.28	62.03	65.80
3	49.66	47.05	57.52	52.74	54.04	55.53	54.33	50.37	53.27	53.43	52.85	52.77	56.79
4	60.24	62.18	62.68	60.61	61.20	60.39	62.25	66.62	63.02	57.10	61.94	61.02	61.63
5	58.73	56.54	58.42	56.00	57.91	53.66	57.59	59.04	58.27	63.76	57.08	52.30	56.07
6	67.03	65.33	66.16	69.17	65.19	66.94	62.60	60.13	64.29	66.77	65.05	63.33	70.14
7	62.14	65.58	64.40	59.08	67.72	64.92	66.07	63.80	62.78	63.97	64.08	65.62	63.89
8	68.84	71.50	66.10	64.10	69.45	69.38	68.96	68.05	62.77	71.48	65.02	68.52	72.59
9	56.39	56.81	58.98	54.72	55.04	58.47	57.13	56.42	58.64	55.30	56.60	58.52	57.67
10	70.74	66.97	69.01	66.62	71.90	65.64	69.84	67.26	68.68	71.12	65.57	68.55	68.00
11	58.41	63.30	59.09	61.02	60.84	61.38	61.22	66.58	66.55	62.03	62.45	58.96	59.62
12	66.42	60.68	62.38	64.89	59.55	65.84	62.51	62.23	62.92	61.48	63.66	57.70	63.90
13	55.63	56.87	55.65	50.10	54.25	54.14	49.60	52.01	53.19	48.67	48.40	54.34	52.24
14	61.73	62.88	61.55	60.48	61.00	59.78	61.58	66.35	59.46	60.15	62.60	63.58	65.18
15	57.63	57.64	60.51	54.27	53.84	63.85	59.82	64.39	60.90	59.71	59.81	59.69	60.49
16	61.10	58.91	56.64	62.80	59.11	65.96	61.82	56.83	62.20	59.63	59.32	58.64	56.83
17	63.17	58.60	61.86	57.86	63.64	56.52	59.48	58.45	58.81	60.06	62.13	63.39	58.73
18	58.00	58.03	57.86	55.33	55.75	60.94	60.63	59.84	60.55	62.17	60.82	60.46	64.98
19	61.62	62.13	58.75	60.84	54.11	63.21	58.11	55.22	55.72	61.69	62.59	58.38	58.01
20	61.98	64.97	61.65	61.99	60.30	60.76	55.30	59.07	59.33	58.88	57.08	57.83	61.02

Table C.6 (cont'd) Data generated at experimental design points (scenario 8)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	57.32	51.48	50.38	54.91	50.89	53.44	49.01	53.35	48.99	52.66	53.40	50.24
2	60.70	64.89	66.65	65.89	64.66	63.44	66.18	64.27	64.30	63.75	62.30	60.08
3	52.61	50.94	53.51	50.24	51.29	55.12	55.69	53.31	55.31	51.93	51.86	51.93
4	58.83	63.68	65.19	62.34	59.29	62.92	68.11	64.09	56.78	61.56	61.74	58.17
5	60.65	56.41	59.50	60.30	52.49	57.94	58.48	54.89	57.68	60.76	58.71	58.20
6	63.61	66.28	65.98	64.70	69.50	65.05	60.26	65.58	66.98	61.60	65.89	65.20
7	69.55	66.99	58.47	58.61	62.54	63.99	63.63	65.46	62.19	62.03	62.37	65.48
8	64.32	66.20	68.35	72.42	68.66	63.33	65.52	73.06	71.99	70.81	64.71	66.23
9	55.76	58.43	56.24	50.50	57.13	58.06	56.52	56.66	58.34	54.18	50.24	60.28
10	69.79	67.97	66.28	69.36	70.74	70.60	67.85	68.05	69.89	68.27	67.38	69.60
11	58.34	61.33	59.31	63.65	62.93	61.96	60.53	63.21	62.62	67.56	61.01	61.76
12	60.80	65.13	64.48	65.23	67.44	58.40	62.89	62.65	62.15	63.88	59.66	66.77
13	53.37	52.81	52.71	50.51	54.41	51.94	50.10	55.36	52.74	49.69	54.27	56.96
14	56.01	60.65	62.06	68.34	63.44	60.11	61.40	62.90	65.97	61.54	65.17	64.19
15	63.57	58.06	61.94	58.96	62.86	62.29	58.86	61.91	62.68	57.76	59.72	58.79
16	60.40	60.86	61.57	61.54	52.84	59.64	62.32	58.22	62.47	59.50	63.82	63.42
17	63.44	59.67	61.07	58.95	64.55	59.61	60.61	55.33	58.78	61.96	58.53	60.76
18	54.77	62.21	61.66	60.01	58.72	61.91	61.10	61.72	63.70	63.02	58.10	64.88
19	63.69	58.61	59.07	62.36	62.32	58.99	55.23	55.64	61.82	56.72	60.67	56.04
20	56.74	56.22	61.96	65.32	57.28	60.66	58.30	58.76	58.60	61.00	64.10	55.24

Table C.7 Estimated model parameters (scenario 5)

$\hat{\boldsymbol{\beta}}$	**Real**		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.72	59.40	80.72	59.40	80.57	58.98	80.72	59.40
$\hat{\beta}_1$	1.00	4.00	1.48	3.99	1.48	3.99	1.11	3.94	1.48	3.99
$\hat{\beta}_2$	4.00	1.00	4.17	1.23	4.17	1.23	4.28	1.21	4.17	1.23
$\hat{\beta}_3$	6.00	3.00	5.99	3.07	5.99	3.07	6.16	3.07	5.99	3.07
$\hat{\beta}_{11}$	-2.00	1.00	-1.93	1.32	-1.93	1.32	-2.04	1.48	-1.93	1.32
$\hat{\beta}_{22}$	3.00	1.00	2.14	0.91	2.14	0.91	2.47	1.02	2.14	0.91
$\hat{\beta}_{33}$	-5.00	-1.00	-5.05	-0.74	-5.05	-0.74	-5.04	-0.60	-5.05	-0.74
$\hat{\beta}_{12}$	2.00	-1.00	1.14	-1.11	1.14	-1.11	1.53	-1.04	1.14	-1.11
$\hat{\beta}_{13}$	12.00	-1.00	11.52	-1.01	11.52	-1.01	11.28	-0.94	11.52	-1.01
$\hat{\beta}_{23}$	-4.00	1.00	-4.86	1.56	-4.86	1.56	-5.20	1.73	-4.86	1.56

Table C.8 Prediction at the center point (scenario 5)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.72	59.40	80.72	59.40	80.57	58.98	80.72	59.40

Table C.9 Prediction at the corner point (scenario 5)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	95.31	68.62	95.31	68.62	95.13	68.85	95.31	68.62

Table C.10 Estimated model parameters (scenario 6)

$\hat{\boldsymbol{\beta}}$	**Real**		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.21	59.73	80.21	59.73	80.16	59.71	80.21	59.73
$\hat{\beta}_1$	1.00	4.00	0.76	4.00	0.76	4.00	0.74	3.98	0.76	4.00
$\hat{\beta}_2$	4.00	1.00	3.49	0.78	3.49	0.78	3.48	0.77	3.49	0.78
$\hat{\beta}_3$	6.00	3.00	5.80	3.01	5.80	3.01	5.82	3.01	5.80	3.01
$\hat{\beta}_{11}$	-2.00	1.00	-2.07	0.83	-2.07	0.83	-2.12	0.84	-2.07	0.83
$\hat{\beta}_{22}$	3.00	1.00	2.46	1.17	2.46	1.17	2.47	1.19	2.46	1.17
$\hat{\beta}_{33}$	-5.00	-1.00	-4.88	-0.86	-4.88	-0.86	-4.85	-0.87	-4.88	-0.86
$\hat{\beta}_{12}$	2.00	-1.00	2.24	-0.85	2.24	-0.85	2.26	-0.88	2.24	-0.85
$\hat{\beta}_{13}$	12.00	-1.00	11.90	-1.12	11.90	-1.12	11.84	-1.12	11.90	-1.12
$\hat{\beta}_{23}$	-4.00	1.00	-3.32	1.05	-3.32	1.05	-3.39	1.06	-3.32	1.05

Table C.11 Prediction at the center point (scenario 6)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.21	59.73	80.21	59.73	80.16	59.71	80.21	59.73

Table C.12 Prediction at the corner point (scenario 6)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	96.58	67.74	96.58	67.74	96.41	67.68	96.58	67.74

Table C.13 Estimated model parameters (scenario 7)

	Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.72	60.06	80.72	60.06	80.57	60.37	80.72	60.06
$\hat{\beta}_1$	1.00	4.00	1.48	4.22	1.48	4.22	1.11	4.00	1.48	4.22
$\hat{\beta}_2$	4.00	1.00	4.17	1.18	4.17	1.18	4.28	1.35	4.17	1.18
$\hat{\beta}_3$	6.00	3.00	5.99	3.03	5.99	3.03	6.16	3.14	5.99	3.03
$\hat{\beta}_{11}$	-2.00	1.00	-1.93	1.18	-1.93	1.18	-2.04	1.05	-1.93	1.18
$\hat{\beta}_{22}$	3.00	1.00	2.14	0.56	2.14	0.56	2.47	0.64	2.14	0.56
$\hat{\beta}_{33}$	-5.00	-1.00	-5.05	-0.90	-5.05	-0.90	-5.04	-1.35	-5.05	-0.90
$\hat{\beta}_{12}$	2.00	-1.00	1.14	-1.45	1.14	-1.45	1.53	-1.07	1.14	-1.45
$\hat{\beta}_{13}$	12.00	-1.00	11.52	-1.23	11.52	-1.23	11.28	-1.30	11.52	-1.23
$\hat{\beta}_{23}$	-4.00	1.00	-4.86	0.86	-4.86	0.86	-5.20	0.65	-4.86	0.86

Table C.14 Prediction at the center point (scenario 7)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.72	60.06	80.72	60.06	80.57	60.37	80.72	60.06

Table C.15 Prediction at the corner point (scenario 7)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	95.31	67.50	95.31	67.50	95.13	67.50	95.31	67.50

Table C.16 Estimated model parameters (scenario 8)

	Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.21	59.97	80.21	59.97	80.16	60.00	80.21	59.97
$\hat{\beta}_1$	1.00	4.00	0.76	3.89	0.76	3.89	0.74	3.83	0.76	3.89
$\hat{\beta}_2$	4.00	1.00	3.49	0.67	3.49	0.67	3.48	0.65	3.49	0.67
$\hat{\beta}_3$	6.00	3.00	5.80	2.91	5.80	2.91	5.82	2.91	5.80	2.91
$\hat{\beta}_{11}$	-2.00	1.00	-2.07	0.89	-2.07	0.89	-2.12	0.85	-2.07	0.89
$\hat{\beta}_{22}$	3.00	1.00	2.46	0.83	2.46	0.83	2.47	0.82	2.46	0.83
$\hat{\beta}_{33}$	-5.00	-1.00	-4.88	-0.88	-4.88	-0.88	-4.85	-0.90	-4.88	-0.88
$\hat{\beta}_{12}$	2.00	-1.00	2.24	-0.82	2.24	-0.82	2.26	-0.85	2.24	-0.82
$\hat{\beta}_{13}$	12.00	-1.00	11.90	-1.10	11.90	-1.10	11.84	-1.13	11.90	-1.10
$\hat{\beta}_{23}$	-4.00	1.00	-3.32	1.34	-3.32	1.34	-3.39	1.30	-3.32	1.34

Table C.17 Prediction at the center point (scenario 8)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.21	59.97	80.21	59.97	80.16	60.00	80.21	59.97

Table C.18 Prediction at the corner point (scenario 8)

Real		**MVR (Variance Known)**		**OLS**		**WLS**		**MVR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	68.00	96.58	67.69	96.58	67.69	96.41	67.48	96.58	67.69

APPENDIX D

GENERATED DATA AND MODEL PARAMETER ESTIMATES UNDER SCENARIOS 9-12: SUR CASE

Table D.1 True mean, variance and covariance values at experimental design points (scenarios 9&10)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	53.00	20.09	7.39	3.65
2	1	-1	-1	49.00	61.00	20.09	7.39	3.65
3	-1	1	-1	87.00	53.00	20.09	7.39	3.65
4	1	1	-1	69.00	61.00	20.09	7.39	3.65
5	-1	-1	1	71.00	59.00	20.09	7.39	3.65
6	1	-1	1	93.00	67.00	20.09	7.39	3.65
7	-1	1	1	67.00	59.00	20.09	7.39	3.65
8	1	1	1	97.00	67.00	20.09	7.39	3.65
9	-1.68	0	0	72.68	53.28	20.09	7.39	3.65
10	1.68	0	0	76.04	66.72	20.09	7.39	3.65
11	0	-1.68	0	81.75	60.00	20.09	7.39	3.65
12	0	1.68	0	95.19	60.00	20.09	7.39	3.65
13	0	0	-1.68	55.81	54.96	20.09	7.39	3.65
14	0	0	1.68	75.97	65.04	20.09	7.39	3.65
15	0	0	0	80.00	60.00	20.09	7.39	3.65
16	0	0	0	80.00	60.00	20.09	7.39	3.65
17	0	0	0	80.00	60.00	20.09	7.39	3.65
18	0	0	0	80.00	60.00	20.09	7.39	3.65
19	0	0	0	80.00	60.00	20.09	7.39	3.65
20	0	0	0	80.00	60.00	20.09	7.39	3.65

Table D.2 True mean, variance and covariance values at experimental design points (scenarios 11&12)

Design Setting	x_1	x_2	x_3	μ_1	μ_2	σ_{11}	σ_{22}	σ_{12}
1	-1	-1	-1	75.00	53.00	20.09	7.39	10.96
2	1	-1	-1	49.00	61.00	20.09	7.39	10.96
3	-1	1	-1	87.00	53.00	20.09	7.39	10.96
4	1	1	-1	69.00	61.00	20.09	7.39	10.96
5	-1	-1	1	71.00	59.00	20.09	7.39	10.96
6	1	-1	1	93.00	67.00	20.09	7.39	10.96
7	-1	1	1	67.00	59.00	20.09	7.39	10.96
8	1	1	1	97.00	67.00	20.09	7.39	10.96
9	-1.68	0	0	72.68	53.28	20.09	7.39	10.96
10	1.68	0	0	76.04	66.72	20.09	7.39	10.96
11	0	-1.68	0	81.75	60.00	20.09	7.39	10.96
12	0	1.68	0	95.19	60.00	20.09	7.39	10.96
13	0	0	-1.68	55.81	54.96	20.09	7.39	10.96
14	0	0	1.68	75.97	65.04	20.09	7.39	10.96
15	0	0	0	80.00	60.00	20.09	7.39	10.96
16	0	0	0	80.00	60.00	20.09	7.39	10.96
17	0	0	0	80.00	60.00	20.09	7.39	10.96
18	0	0	0	80.00	60.00	20.09	7.39	10.96
19	0	0	0	80.00	60.00	20.09	7.39	10.96
20	0	0	0	80.00	60.00	20.09	7.39	10.96

Table D.3 Data generated at experimental design points (scenario 9)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	73.06	67.54	75.56	76.29	69.86	55.74	54.73	53.00	54.08	52.52
2	48.16	52.25	46.36	58.78	48.39	61.14	64.36	60.67	62.53	58.73
3	88.32	81.01	90.20	94.28	83.90	55.46	55.16	49.45	50.59	53.92
4	67.21	72.09	72.66	72.19	74.78	62.41	64.65	58.55	61.53	61.65
5	63.81	72.15	66.27	77.34	67.39	59.06	59.78	55.75	54.53	58.19
6	88.47	95.75	95.28	100.58	95.65	64.51	68.49	64.80	68.33	67.36
7	67.00	65.58	71.91	58.60	68.92	61.32	60.64	61.39	57.58	61.10
8	99.55	95.85	95.31	95.67	90.39	66.86	67.10	67.51	70.50	64.89
9	75.47	76.26	76.89	68.23	73.63	54.41	51.32	52.12	55.28	53.11
10	77.78	76.43	73.19	73.53	78.02	64.57	68.82	67.68	64.13	66.39
11	76.42	71.88	86.17	79.42	83.21	59.64	58.26	58.20	57.12	59.30
12	89.87	90.45	101.79	95.44	89.73	58.93	56.21	57.70	59.37	61.48
13	56.38	58.75	50.57	53.74	54.63	51.92	52.07	56.42	54.61	53.07
14	79.58	77.01	71.53	81.97	77.27	69.53	68.18	62.46	62.78	65.09
15	78.52	76.22	82.23	86.67	77.55	57.53	58.67	62.13	59.00	56.44
16	79.46	79.71	82.17	77.33	79.33	58.77	59.74	64.38	57.94	56.38
17	82.10	75.95	80.16	77.19	82.40	61.82	58.73	54.70	59.83	64.57
18	84.56	72.92	79.65	76.95	75.41	57.63	59.46	58.82	59.59	58.21
19	77.92	81.66	83.26	89.47	73.92	56.97	62.99	59.58	58.14	59.71
20	86.96	83.17	88.77	82.26	88.36	60.39	57.62	61.05	63.50	58.63

Table D.4 Data generated at experimental design points (scenario 10)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	73.06	67.54	75.56	76.29	69.86	80.34	80.33	74.83	76.47	75.78	74.16	78.25	72.36
2	44.47	51.75	51.28	56.58	51.65	46.12	50.70	44.48	48.91	48.78	49.00	47.58	53.91
3	81.68	77.13	91.42	84.68	88.47	88.05	87.10	82.50	82.76	85.32	81.69	82.27	93.60
4	68.46	68.71	71.17	66.33	68.33	67.05	68.64	75.88	66.28	62.96	71.10	64.95	69.16
5	73.85	68.30	73.47	66.07	71.39	62.02	68.79	73.07	69.56	76.54	68.17	60.58	65.48
6	97.44	93.98	94.17	98.44	91.77	92.40	87.31	85.54	89.85	94.26	90.57	87.02	97.81
7	62.98	67.61	66.38	61.79	72.31	66.93	69.40	63.79	64.06	68.41	67.48	75.28	65.77
8	98.98	102.74	94.77	91.99	100.62	97.18	93.61	96.60	88.00	101.86	92.60	93.91	103.00
9	72.35	73.93	78.83	73.48	70.25	80.00	76.37	73.71	75.69	70.40	76.51	73.88	75.48
10	75.51	76.79	73.79	72.88	78.31	74.15	77.06	71.74	75.38	79.37	72.04	76.66	74.98
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	60.93	62.76	62.01	52.41	57.79	59.89	50.99	56.71	59.23	50.03	51.54	59.30	55.78
14	75.58	77.43	74.47	74.52	74.25	71.70	77.01	81.50	73.38	73.72	79.21	76.15	82.88
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table D.4 (cont'd) Data generated at experimental design points (scenario 10)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	84.78	74.39	75.51	79.78	75.27	74.57	71.27	76.32	69.01	78.20	82.28	71.90
2	40.60	50.92	53.01	52.28	51.59	49.18	52.03	51.55	47.85	47.31	47.67	42.39
3	87.25	81.54	86.82	81.94	80.95	85.83	91.27	87.58	89.94	81.77	84.94	85.82
4	66.19	71.40	71.48	68.09	59.79	69.59	76.14	73.56	61.92	68.65	65.95	64.41
5	75.73	70.49	72.70	75.23	61.50	68.11	67.84	66.44	70.18	77.82	70.83	76.50
6	89.81	92.95	93.00	91.88	94.78	91.82	85.54	88.39	94.09	87.37	91.44	88.78
7	76.92	73.76	58.28	59.47	64.43	66.17	67.04	70.75	63.76	63.77	66.10	66.91
8	92.93	95.15	94.73	104.26	97.36	92.16	91.96	104.78	105.68	104.33	91.37	96.04
9	67.98	79.56	74.62	64.08	74.78	78.39	75.54	78.86	78.59	68.60	62.34	80.69
10	75.70	74.43	66.72	75.39	82.28	78.96	74.35	73.07	77.15	74.32	73.67	76.28
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	58.16	61.92	57.97	52.28	59.18	55.06	52.15	65.19	56.17	51.61	58.66	63.35
14	68.34	71.34	72.55	85.72	77.90	73.98	76.10	74.55	80.35	76.05	79.63	79.12
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table D.4 (cont'd) Data generated at experimental design points (scenario 10)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	54.87	54.89	48.97	49.50	53.55	52.93	55.76	55.08	55.11	56.49	54.58	56.68	49.40
2	59.57	61.81	62.23	66.12	60.57	62.09	63.38	62.62	58.41	61.51	61.62	58.13	59.97
3	48.89	47.78	56.22	52.61	51.59	55.28	53.62	49.61	55.70	53.45	55.87	55.09	52.43
4	57.70	61.70	60.28	60.66	59.92	59.44	61.90	64.14	65.98	56.38	58.73	62.95	60.02
5	57.71	58.53	57.42	59.63	58.42	58.61	60.33	59.17	61.04	66.00	59.85	57.07	60.36
6	64.76	64.53	66.17	68.44	66.47	69.65	65.33	61.71	66.45	67.41	67.38	67.21	71.19
7	58.99	61.85	60.50	53.51	61.77	61.09	61.09	61.81	59.31	57.51	58.70	54.16	60.00
8	66.84	68.84	65.11	63.55	66.50	69.84	72.54	67.52	64.67	69.70	64.94	71.27	70.96
9	54.24	53.56	53.35	49.45	53.41	51.05	51.78	52.93	55.79	53.84	50.49	57.34	53.87
10	69.88	60.32	67.83	63.53	69.58	60.09	66.33	66.09	65.50	66.80	62.07	63.91	64.41
11	60.58	61.94	61.52	62.73	60.00	59.39	60.53	64.00	64.48	59.10	62.44	58.90	58.75
12	61.17	57.95	61.25	63.60	55.91	60.39	56.89	60.89	60.57	57.85	58.49	56.08	61.83
13	57.43	58.27	56.36	53.93	57.58	55.20	54.28	53.76	53.80	53.21	51.10	56.24	55.22
14	64.37	65.01	65.10	62.70	64.11	64.03	62.58	68.48	61.63	62.79	62.60	67.83	64.53
15	56.51	58.61	59.82	55.71	53.65	59.29	59.93	57.67	63.08	58.58	55.40	60.14	63.43
16	62.47	56.00	56.70	62.44	57.56	60.65	62.12	58.99	63.07	56.93	60.83	55.95	55.77
17	63.49	60.07	60.98	60.18	63.89	62.02	57.57	59.93	60.90	59.44	66.20	63.01	57.71
18	59.84	56.20	58.96	57.33	54.78	59.40	58.86	61.53	60.93	62.66	60.90	59.83	61.46
19	61.55	62.09	60.42	58.05	57.28	62.04	55.88	56.86	56.20	62.77	64.66	61.02	57.69
20	59.87	62.87	57.13	60.21	59.16	61.34	56.52	59.87	58.63	56.52	58.18	58.27	59.70

Table D.4 (cont'd) Data generated at experimental design points (scenario 10)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	54.73	52.48	48.93	54.54	50.31	56.59	50.23	54.61	52.48	51.19	48.70	52.28
2	62.28	61.01	62.74	61.82	59.82	59.58	62.70	59.00	62.82	62.17	58.63	59.11
3	49.70	51.82	52.11	49.89	53.19	56.65	52.36	50.91	52.90	53.77	50.41	49.67
4	56.91	62.25	65.48	62.67	64.40	62.42	67.13	60.95	56.76	60.39	63.53	57.27
5	60.01	56.04	60.57	59.76	56.55	61.78	63.26	56.81	59.12	58.15	60.73	53.87
6	65.00	67.67	66.97	65.29	72.86	66.12	61.99	70.75	68.04	63.07	68.33	69.52
7	61.11	58.70	55.72	54.83	58.41	59.83	58.15	58.39	58.32	57.96	56.35	62.33
8	63.08	64.93	70.06	69.33	68.09	61.69	66.67	70.19	66.93	65.73	65.49	64.09
9	57.28	51.40	51.60	49.73	53.39	51.79	51.30	48.24	52.18	53.21	50.92	54.30
10	67.61	64.91	69.01	66.97	63.03	66.07	64.72	66.45	66.35	65.68	64.39	66.60
11	60.26	62.11	58.14	57.54	60.48	61.49	59.98	64.16	59.77	63.89	58.23	57.43
12	58.22	59.88	57.22	60.93	66.89	58.60	56.33	59.93	56.06	60.12	54.67	62.34
13	55.28	50.24	54.03	54.96	56.53	55.29	54.20	52.51	55.91	53.86	56.74	57.88
14	59.18	66.31	68.16	68.56	65.75	62.45	63.11	67.97	68.82	63.48	67.80	66.18
15	61.31	59.71	60.59	60.03	62.89	61.16	61.28	61.75	61.18	59.87	57.75	57.52
16	60.78	59.98	58.04	59.87	56.33	57.91	61.32	56.13	61.51	55.38	62.44	61.89
17	62.93	61.43	62.03	55.88	64.90	56.33	62.64	56.00	60.44	62.77	61.31	60.33
18	58.89	63.30	62.33	57.02	59.84	60.15	61.62	59.91	63.73	60.61	56.14	64.69
19	61.73	59.04	57.81	61.55	61.02	57.17	56.91	57.94	62.05	56.16	58.91	57.62
20	58.25	55.25	63.06	64.69	58.81	58.60	59.90	58.71	59.68	56.47	65.07	59.13

Table D.5 Data generated at experimental design points (scenario 11)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$
1	73.06	67.54	75.56	76.29	69.86	53.35	50.33	53.26	54.09	50.40
2	48.16	52.25	46.36	58.78	48.39	60.68	64.04	59.63	66.23	59.68
3	88.32	81.01	90.20	94.28	83.90	54.74	51.22	52.86	55.26	51.98
4	67.21	72.09	72.66	72.19	74.78	60.81	64.10	61.57	62.72	63.97
5	63.81	72.15	66.27	77.34	67.39	55.70	59.89	55.32	59.89	56.96
6	88.47	95.75	95.28	100.58	95.65	63.76	68.95	67.05	71.12	68.39
7	67.00	65.58	71.91	58.60	68.92	60.06	59.09	62.36	54.46	60.85
8	99.55	95.85	95.31	95.67	90.39	68.11	66.51	66.45	67.99	62.98
9	75.47	76.26	76.89	68.23	73.63	55.09	54.04	54.70	52.14	53.64
10	77.78	76.43	73.19	73.53	78.02	66.55	67.86	65.84	64.38	67.49
11	76.42	71.88	86.17	79.42	83.21	57.37	54.64	61.22	57.61	60.36
12	89.87	90.45	101.79	95.44	89.73	57.05	56.08	62.00	59.83	58.15
13	56.38	58.75	50.57	53.74	54.63	53.84	55.00	53.21	53.85	53.55
14	79.58	77.01	71.53	81.97	77.27	68.76	66.96	61.81	66.79	65.66
15	78.52	76.22	82.23	86.67	77.55	58.19	57.64	62.00	62.63	57.24
16	79.46	79.71	82.17	77.33	79.33	59.19	59.75	63.01	57.82	58.04
17	82.10	75.95	80.16	77.19	82.40	61.80	57.55	57.65	58.62	63.20
18	84.56	72.92	79.65	76.95	75.41	61.03	56.48	59.30	58.40	57.06
19	77.92	81.66	83.26	89.47	73.92	57.65	62.14	61.32	63.53	57.05
20	86.96	83.17	88.77	82.26	88.36	63.40	60.38	64.54	62.64	63.24

Table D.6 Data generated at experimental design points (scenario 12)

Design Setting	$y_{1,1}$	$y_{1,2}$	$y_{1,3}$	$y_{1,4}$	$y_{1,5}$	$y_{1,6}$	$y_{1,7}$	$y_{1,8}$	$y_{1,9}$	$y_{1,10}$	$y_{1,11}$	$y_{1,12}$	$y_{1,13}$
1	73.06	67.54	75.56	76.29	69.86	80.34	80.33	74.83	76.47	75.78	74.16	78.25	72.36
2	44.47	51.75	51.28	56.58	51.65	46.12	50.70	44.48	48.91	48.78	49.00	47.58	53.91
3	81.68	77.13	91.42	84.68	88.47	88.05	87.10	82.50	82.76	85.32	81.69	82.27	93.60
4	68.46	68.71	71.17	66.33	68.33	67.05	68.64	75.88	66.28	62.96	71.10	64.95	69.16
5	73.85	68.30	73.47	66.07	71.39	62.02	68.79	73.07	69.56	76.54	68.17	60.58	65.48
6	97.44	93.98	94.17	98.44	91.77	92.40	87.31	85.54	89.85	94.26	90.57	87.02	97.81
7	62.98	67.61	66.38	61.79	72.31	66.93	69.40	63.79	64.06	68.41	67.48	75.28	65.77
8	98.98	102.74	94.77	91.99	100.62	97.18	93.61	96.60	88.00	101.86	92.60	93.91	103.00
9	72.35	73.93	78.83	73.48	70.25	80.00	76.37	73.71	75.69	70.40	76.51	73.88	75.48
10	75.51	76.79	73.79	72.88	78.31	74.15	77.06	71.74	75.38	79.37	72.04	76.66	74.98
11	75.28	84.49	75.82	78.78	81.09	82.86	81.40	89.54	89.02	84.55	82.16	78.13	79.68
12	98.17	88.95	89.36	92.48	88.52	97.69	93.94	89.39	91.21	90.77	94.87	84.37	92.08
13	60.93	62.76	62.01	52.41	57.79	59.89	50.99	56.71	59.23	50.03	51.54	59.30	55.78
14	75.58	77.43	74.47	74.52	74.25	71.70	77.01	81.50	73.38	73.72	79.21	76.15	82.88
15	78.33	76.27	81.29	71.85	72.95	89.03	79.68	91.78	78.91	80.78	84.14	79.20	77.66
16	79.94	81.59	75.99	83.64	80.49	92.24	81.84	74.14	81.72	82.24	77.71	81.05	77.32
17	83.40	76.90	83.05	75.19	84.03	70.48	81.28	76.71	76.53	80.68	78.49	84.35	79.52
18	75.85	79.50	76.40	72.54	75.96	82.64	82.48	78.14	80.28	82.05	80.89	81.15	89.33
19	81.98	82.53	76.89	83.74	69.97	84.92	79.99	72.76	74.49	80.93	80.99	75.49	77.97
20	84.41	87.90	86.40	84.09	81.46	80.31	73.28	78.13	79.91	81.02	75.48	77.02	82.50

Table D.6 (cont'd) Data generated at experimental design points (scenario 12)

Design Setting	$y_{1,14}$	$y_{1,15}$	$y_{1,16}$	$y_{1,17}$	$y_{1,18}$	$y_{1,19}$	$y_{1,20}$	$y_{1,21}$	$y_{1,22}$	$y_{1,23}$	$y_{1,24}$	$y_{1,25}$
1	84.78	74.39	75.51	79.78	75.27	74.57	71.27	76.32	69.01	78.20	82.28	71.90
2	40.60	50.92	53.01	52.28	51.59	49.18	52.03	51.55	47.85	47.31	47.67	42.39
3	87.25	81.54	86.82	81.94	80.95	85.83	91.27	87.58	89.94	81.77	84.94	85.82
4	66.19	71.40	71.48	68.09	59.79	69.59	76.14	73.56	61.92	68.65	65.95	64.41
5	75.73	70.49	72.70	75.23	61.50	68.11	67.84	66.44	70.18	77.82	70.83	76.50
6	89.81	92.95	93.00	91.88	94.78	91.82	85.54	88.39	94.09	87.37	91.44	88.78
7	76.92	73.76	58.28	59.47	64.43	66.17	67.04	70.75	63.76	63.77	66.10	66.91
8	92.93	95.15	94.73	104.26	97.36	92.16	91.96	104.78	105.68	104.33	91.37	96.04
9	67.98	79.56	74.62	64.08	74.78	78.39	75.54	78.86	78.59	68.60	62.34	80.69
10	75.70	74.43	66.72	75.39	82.28	78.96	74.35	73.07	77.15	74.32	73.67	76.28
11	75.45	80.07	79.64	89.60	85.12	82.04	80.44	82.12	85.18	91.77	83.21	85.62
12	88.95	96.66	97.87	95.85	94.73	83.38	95.31	91.26	94.00	93.72	90.00	97.79
13	58.16	61.92	57.97	52.28	59.18	55.06	52.15	65.19	56.17	51.61	58.66	63.35
14	68.34	71.34	72.55	85.72	77.90	73.98	76.10	74.55	80.35	76.05	79.63	79.12
15	86.42	76.10	83.62	77.71	83.33	83.80	76.28	82.39	84.63	75.29	81.62	79.84
16	80.09	81.88	85.34	83.46	68.15	81.28	83.70	79.96	83.85	83.47	85.85	85.52
17	84.54	77.87	80.31	81.79	85.00	82.78	78.71	73.85	76.93	81.49	75.53	81.31
18	69.79	81.52	81.30	82.97	77.40	83.98	80.77	83.80	84.32	85.92	79.71	85.90
19	86.27	77.93	80.15	83.58	84.02	80.62	72.74	72.62	81.92	76.70	82.53	73.80
20	74.67	76.52	81.21	86.88	75.28	82.80	76.43	78.59	77.30	85.64	83.85	70.56

Table D.6 (cont'd) Data generated at experimental design points (scenario 12)

Design Setting	$y_{2,1}$	$y_{2,2}$	$y_{2,3}$	$y_{2,4}$	$y_{2,5}$	$y_{2,6}$	$y_{2,7}$	$y_{2,8}$	$y_{2,9}$	$y_{2,10}$	$y_{2,11}$	$y_{2,12}$	$y_{2,13}$
1	52.96	50.41	51.42	52.00	50.87	55.44	56.73	53.87	54.64	54.96	53.34	56.19	50.14
2	58.25	62.64	62.62	66.85	62.03	60.16	62.88	59.65	59.78	61.13	61.28	59.03	62.80
3	48.66	46.05	56.52	51.74	53.04	54.53	53.33	49.37	52.27	52.43	51.85	51.77	55.79
4	59.24	61.18	61.68	59.61	60.20	59.39	61.25	65.62	62.02	56.10	60.94	60.02	60.63
5	59.73	57.54	59.42	57.00	58.91	54.66	58.59	60.04	59.27	64.76	58.08	53.30	57.07
6	68.03	66.33	67.16	70.17	66.19	67.94	63.60	61.13	65.29	67.77	66.05	64.33	71.14
7	57.14	60.58	59.40	54.08	62.72	59.92	61.07	58.80	57.78	58.97	59.08	60.62	58.89
8	67.84	70.50	65.10	63.10	68.45	68.38	67.96	67.05	61.77	70.48	64.02	67.52	71.59
9	53.57	53.99	56.16	51.90	52.22	55.65	54.30	53.60	55.82	52.48	53.78	55.69	54.85
10	67.92	64.15	66.19	63.80	69.08	62.82	67.02	64.44	65.86	68.30	62.75	65.73	65.18
11	57.27	62.16	57.95	59.87	59.69	60.23	60.08	65.43	65.41	60.89	61.31	57.82	58.47
12	61.92	56.18	57.88	60.39	55.05	61.34	58.01	57.72	58.42	56.97	59.16	53.20	59.40
13	58.46	59.69	58.47	52.92	57.07	56.96	52.42	54.83	56.01	51.49	51.22	57.16	55.07
14	64.56	65.70	64.37	63.30	63.82	62.60	64.40	69.17	62.28	62.97	65.42	66.40	68.00
15	57.63	57.64	60.51	54.27	53.84	63.85	59.82	64.39	60.90	59.71	59.81	59.69	60.49
16	61.10	58.91	56.64	62.80	59.11	65.96	61.82	56.83	62.20	59.63	59.32	58.64	56.83
17	63.17	58.60	61.86	57.86	63.64	56.52	59.48	58.45	58.81	60.06	62.13	63.39	58.73
18	58.00	58.03	57.86	55.33	55.75	60.94	60.63	59.84	60.55	62.17	60.82	60.46	64.98
19	61.62	62.13	58.75	60.84	54.11	63.21	58.11	55.22	55.72	61.69	62.59	58.38	58.01
20	61.98	64.97	61.65	61.99	60.30	60.76	55.30	59.07	59.33	58.88	57.08	57.83	61.02

Table D.6 (cont'd) Data generated at experimental design points (scenario 12)

Design Setting	$y_{2,14}$	$y_{2,15}$	$y_{2,16}$	$y_{2,17}$	$y_{2,18}$	$y_{2,19}$	$y_{2,20}$	$y_{2,21}$	$y_{2,22}$	$y_{2,23}$	$y_{2,24}$	$y_{2,25}$
1	58.32	52.48	51.38	55.91	51.89	54.44	50.01	54.35	49.99	53.66	54.40	51.24
2	57.70	61.89	63.65	62.89	61.66	60.44	63.18	61.27	61.30	60.75	59.30	57.08
3	51.61	49.94	52.51	49.24	50.29	54.12	54.69	52.31	54.31	50.93	50.86	50.93
4	57.83	62.68	64.19	61.34	58.29	61.92	67.11	63.09	55.78	60.56	60.74	57.17
5	61.65	57.41	60.50	61.30	53.49	58.94	59.48	55.89	58.68	61.76	59.71	59.20
6	64.61	67.28	66.98	65.70	70.50	66.05	61.26	66.58	67.98	62.60	66.89	66.20
7	64.55	61.99	53.47	53.61	57.54	58.99	58.63	60.46	57.19	57.03	57.37	60.48
8	63.32	65.20	67.35	71.42	67.66	62.33	64.52	72.06	70.99	69.81	63.71	65.23
9	52.93	55.60	53.42	47.68	54.30	55.24	53.70	53.84	55.52	51.36	47.42	57.46
10	66.97	65.15	63.46	66.53	67.92	67.78	65.02	65.22	67.07	65.45	64.56	66.78
11	57.20	60.19	58.17	62.51	61.78	60.81	59.38	62.07	61.48	66.41	59.87	60.62
12	56.30	60.63	59.97	60.73	62.94	53.90	58.38	58.15	57.65	59.37	55.16	62.27
13	56.19	55.63	55.53	53.33	57.24	54.76	52.92	58.18	55.56	52.51	57.09	59.78
14	58.83	63.47	64.88	71.16	66.26	62.94	64.22	65.72	68.80	64.36	68.00	67.02
15	63.57	58.06	61.94	58.96	62.86	62.29	58.86	61.91	62.68	57.76	59.72	58.79
16	60.40	60.86	61.57	61.54	52.84	59.64	62.32	58.22	62.47	59.50	63.82	63.42
17	63.44	59.67	61.07	58.95	64.55	59.61	60.61	55.33	58.78	61.96	58.53	60.76
18	54.77	62.21	61.66	60.01	58.72	61.91	61.10	61.72	63.70	63.02	58.10	64.88
19	63.69	58.61	59.07	62.36	62.32	58.99	55.23	55.64	61.82	56.72	60.67	56.04
20	56.74	56.22	61.96	65.32	57.28	60.66	58.30	58.76	58.60	61.00	64.10	55.24

Table D.7 Estimated model parameters (scenario 9)

$\hat{\boldsymbol{\beta}}$	**Real**		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.89	59.74	80.72	59.74	80.57	59.48	80.78	59.74
$\hat{\beta}_1$	1.00	4.00	1.48	3.99	1.48	3.99	1.11	3.75	1.48	3.99
$\hat{\beta}_2$	4.00	-	4.05	-	4.17	-	4.28	-	4.13	-
$\hat{\beta}_3$	6.00	3.00	5.99	3.07	5.99	3.07	6.16	2.99	5.99	3.07
$\hat{\beta}_{11}$	-2.00	-	-2.09	-	-1.93	-	-2.04	-	-1.99	-
$\hat{\beta}_{22}$	3.00	-	2.19	-	2.14	-	2.47	-	2.16	-
$\hat{\beta}_{33}$	-5.00	-	-5.18	-	-5.05	-	-5.04	-	-5.10	-
$\hat{\beta}_{12}$	2.00	-	1.20	-	1.14	-	1.53	-	1.16	-
$\hat{\beta}_{13}$	12.00	-	11.52	-	11.52	-	11.28	-	11.52	-
$\hat{\beta}_{23}$	-4.00	-	-5.13	-	-4.86	-	-5.20	-	-4.96	-

Table D.8 Prediction at the center point (scenario 9)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.89	59.74	80.72	59.74	80.57	59.48	80.78	59.74

Table D.9 Prediction at the corner point (scenario 9)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	67.00	94.91	66.80	95.31	66.80	95.13	66.23	95.17	66.80

Table D.10 Estimated model parameters (scenario 10)

$\hat{\boldsymbol{\beta}}$	**Real**		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.25	59.83	80.21	59.83	80.16	59.84	80.25	59.83
$\hat{\beta}_1$	1.00	4.00	0.76	4.00	0.76	4.00	0.74	4.02	0.76	4.00
$\hat{\beta}_2$	4.00	-	3.60	-	3.49	-	3.48	-	3.60	-
$\hat{\beta}_3$	6.00	3.00	5.80	3.01	5.80	3.01	5.82	2.98	5.80	3.01
$\hat{\beta}_{11}$	-2.00	-	-1.98	-	-2.07	-	-2.12	-	-1.99	-
$\hat{\beta}_{22}$	3.00	-	2.38	-	2.46	-	2.47	-	2.38	-
$\hat{\beta}_{33}$	-5.00	-	-4.95	-	-4.88	-	-4.85	-	-4.95	-
$\hat{\beta}_{12}$	2.00	-	2.16	-	2.24	-	2.26	-	2.17	-
$\hat{\beta}_{13}$	12.00	-	11.96	-	11.90	-	11.84	-	11.95	-
$\hat{\beta}_{23}$	-4.00	-	-3.34	-	-3.32	-	-3.39	-	-3.34	-

Table D.11 Prediction at the center point (scenario 10)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.25	59.83	80.21	59.83	80.16	59.84	80.25	59.83

Table D.12 Prediction at the corner point (scenario 10)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	67.00	96.63	66.83	96.58	66.83	96.41	66.84	96.63	66.83

Table D.13 Estimated model parameters (scenario 11)

	Real		SUR (Variance Known)		OLS		WLS		SUR	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.56	59.95	80.72	59.95	80.57	60.03	80.55	59.95
$\hat{\beta}_1$	1.00	4.00	1.48	4.22	1.48	4.22	1.11	4.03	1.48	4.22
$\hat{\beta}_2$	4.00	-	3.89	-	4.17	-	4.28	-	3.88	-
$\hat{\beta}_3$	6.00	3.00	5.99	3.03	5.99	3.03	6.16	3.38	5.99	3.03
$\hat{\beta}_{11}$	-2.00	-	-2.20	-	-1.93	-	-2.04	-	-2.21	-
$\hat{\beta}_{22}$	3.00	-	2.80	-	2.14	-	2.47	-	2.84	-
$\hat{\beta}_{33}$	-5.00	-	-5.20	-	-5.05	-	-5.04	-	-5.21	-
$\hat{\beta}_{12}$	2.00	-	1.81	-	1.14	-	1.53	-	1.85	-
$\hat{\beta}_{13}$	12.00	-	11.86	-	11.52	-	11.28	-	11.88	-
$\hat{\beta}_{23}$	-4.00	-	-4.65	-	-4.86	-	-5.20	-	-4.63	-

Table D.14 Prediction at the center point (scenario 11)

Real		SUR (Variance Known)		OLS		WLS		SUR	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.56	59.95	80.72	59.95	80.57	60.03	80.55	59.95

Table D.15 Prediction at the corner point (scenario 11)

Real		SUR (Variance Known)		OLS		WLS		SUR	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	67.00	96.34	67.19	95.31	67.19	95.13	67.45	96.40	67.19

Table D.16 Estimated model parameters (scenario 12)

	Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{\boldsymbol{\beta}}$	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2	For y_1	For y_2
$\hat{\beta}_0$	80.00	60.00	80.04	59.86	80.21	59.86	80.16	59.84	80.04	59.86
$\hat{\beta}_1$	1.00	4.00	0.76	3.89	0.76	3.89	0.74	3.82	0.76	3.89
$\hat{\beta}_2$	4.00	-	3.99	-	3.49	-	3.48	-	3.98	-
$\hat{\beta}_3$	6.00	3.00	5.80	2.91	5.80	2.91	5.82	2.89	5.80	2.91
$\hat{\beta}_{11}$	-2.00	-	-1.91	-	-2.07	-	-2.12	-	-1.91	-
$\hat{\beta}_{22}$	3.00	-	2.72	-	2.46	-	2.47	-	2.72	-
$\hat{\beta}_{33}$	-5.00	-	-5.06	-	-4.88	-	-4.85	-	-5.06	-
$\hat{\beta}_{12}$	2.00	-	1.97	-	2.24	-	2.26	-	1.98	-
$\hat{\beta}_{13}$	12.00	-	12.05	-	11.90	-	11.84	-	12.05	-
$\hat{\beta}_{23}$	-4.00	-	-3.82	-	-3.32	-	-3.39	-	-3.81	-

Table D.17 Prediction at the center point (scenario 12)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
80.00	60.00	80.04	59.86	80.21	59.86	80.16	59.84	80.04	59.86

Table D.18 Prediction at the corner point (scenario 12)

Real		**SUR (Variance Known)**		**OLS**		**WLS**		**SUR**	
$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$	$\hat{y}_1$	$\hat{y}_2$
97.00	67.00	96.54	66.66	96.58	66.66	96.41	66.55	96.54	66.66

APPENDIX E

DATA USED TO CONDUCT ANOVA AND RESULTS

Table E.1 Data used in ANOVA

No.	Number of replications n	Correlation Coefficient, ρ	Heterosce-dasticity (0: No, 1: Yes)	Set of Predictors of the Responses (0: Same, 1: Different)	Position of the Design Point (0: Center, 1: Corner)
1	5	0	0	0	0
2	5	0	0	0	1
3	25	0	0	0	0
4	25	0	0	0	1
5	5	0	1	0	0
6	5	0	1	0	1
7	25	0	1	0	0
8	25	0	1	0	1
9	5	0.3	0	0	0
10	5	0.3	0	0	1
11	25	0.3	0	0	0
12	25	0.3	0	0	1
13	5	0.9	0	0	0
14	5	0.9	0	0	1
15	25	0.9	0	0	0
16	25	0.9	0	0	1
17	5	0.3	0	1	0
18	5	0.3	0	1	1
19	25	0.3	0	1	0
20	25	0.3	0	1	1
21	5	0.9	0	1	0
22	5	0.9	0	1	1
23	25	0.9	0	1	0
24	25	0.9	0	1	1

Table E.1 Data used in ANOVA (cont'd)

No.	OLS Applicability (0: Not Applicable, 1: Applicable)	WLS Applicability (0: Not App., 1: App.)	SUR Applicability (0: Not App., 1: App.)	d_H BLUE	d_H OLS	d_H WLS	d_H SUR
1	1	0	0	0.159	0.196	0.936	0.264
2	1	0	0	0.242	0.272	0.863	0.319
3	1	0	0	0.063	0.091	0.959	0.099
4	1	0	0	0.058	0.088	0.906	0.096
5	0	1	0	0.16	0.489	0.938	0.547
6	0	1	0	0.261	0.993	0.506	0.965
7	0	1	0	0.057	0.465	0.957	0.474
8	0	1	0	0.022	0.989	0.473	0.984
9	0	0	1	0.159	0.256	0.938	0.264
10	0	0	1	0.242	0.308	0.854	0.319
11	0	0	1	0.063	0.171	0.95	0.099
12	0	0	1	0.058	0.172	0.897	0.096
13	0	0	1	0.159	0.705	0.829	0.265
14	0	0	1	0.242	0.718	0.795	0.32
15	0	0	1	0.063	0.709	0.865	0.099
16	0	0	1	0.058	0.71	0.829	0.096
17	0	0	1	0.126	0.23	0.914	0.222
18	0	0	1	0.22	0.27	0.846	0.274
19	0	0	1	0.051	0.165	0.951	0.087
20	0	0	1	0.045	0.167	0.909	0.084
21	0	0	1	0.159	0.703	0.831	0.209
22	0	0	1	0.229	0.719	0.877	0.255
23	0	0	1	0.067	0.709	0.869	0.082
24	0	0	1	0.064	0.709	0.83	0.079

Table E.1 Data used in ANOVA (cont'd)

No.	diffOLS= d_HOLS - d_HBLUE	diffWLS= d_HWLS-d_HBLUE	diffSUR= d_HSUR-d_HBLUE
1	0.037	0.777	0.105
2	0.03	0.621	0.077
3	0.028	0.896	0.036
4	0.03	0.848	0.038
5	0.329	0.778	0.387
6	0.732	0.245	0.704
7	0.408	0.9	0.417
8	0.967	0.451	0.962
9	0.097	0.779	0.105
10	0.066	0.612	0.077
11	0.108	0.887	0.036
12	0.114	0.839	0.038
13	0.546	0.67	0.106
14	0.476	0.553	0.078
15	0.646	0.802	0.036
16	0.652	0.771	0.038
17	0.104	0.788	0.096
18	0.05	0.626	0.054
19	0.114	0.9	0.036
20	0.122	0.864	0.039
21	0.544	0.672	0.05
22	0.49	0.648	0.026
23	0.642	0.802	0.015
24	0.645	0.766	0.015

Table E.2 Result of ANOVA analysis for logarithm of diffOLS values

General Linear Model: logdiffOLS versus n, rho, heteroscedas, set of predi, position of , ...

```
Method

Factor coding  (-1, 0, +1)

Stepwise Selection of Terms

α to enter = 0.15, α to remove = 0.15

Factor Information

Factor             Type   Levels  Values
n                  Fixed       2  5, 25
rho                Fixed       3  0.0, 0.3, 0.9
OLSapplicability   Fixed       2  0, 1

Analysis of Variance

Source               DF   Adj SS   Adj MS  F-Value  P-Value
  n                   1  0.06056  0.06056     4.72    0.043
  rho                 2  2.96238  1.48119   115.37    0.000
  OLSapplicability    1  3.13525  3.13525   244.20    0.000
Error                19  0.24394  0.01284
Total                23  6.26504

Model Summary

       S    R-sq  R-sq(adj)  R-sq(pred)
0.113309  96.11%     95.29%      92.97%

Coefficients

Term                 Coef  SE Coef  T-Value  P-Value   VIF
Constant          -1.1346   0.0353   -32.11    0.000
n
  5               -0.0502   0.0231    -2.17    0.043  1.00
rho
  0.0              0.2530   0.0422     5.99    0.000  2.22
  0.3             -0.5219   0.0353   -14.77    0.000  1.56
OLSapplicability
  0                0.6260   0.0401    15.63    0.000  1.67
```

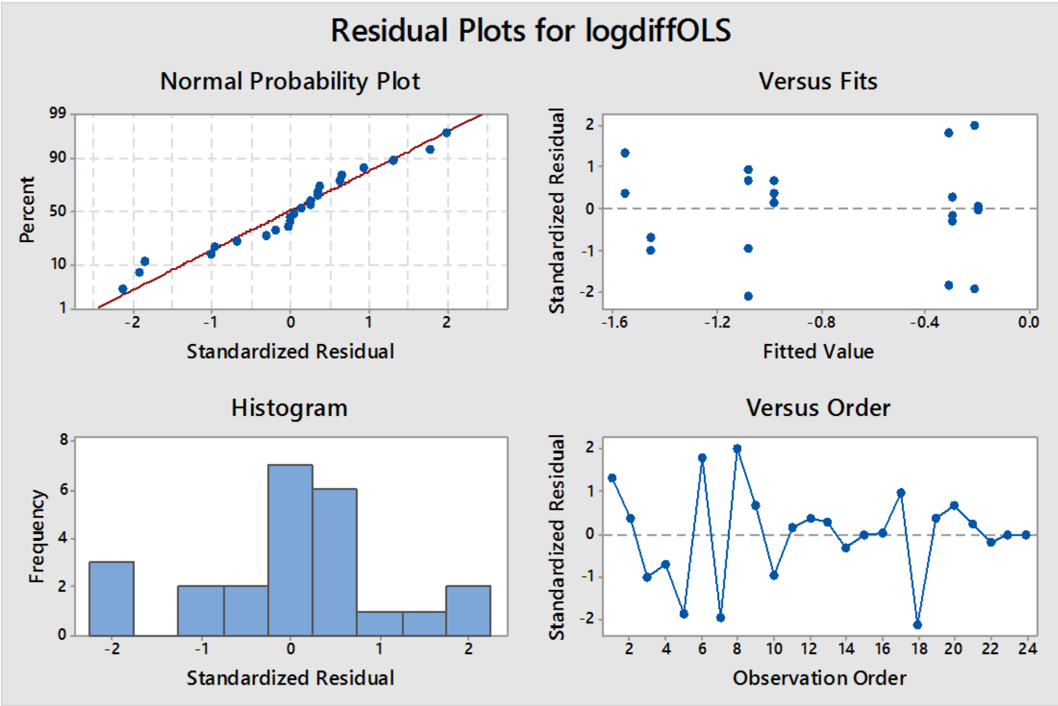

Figure E.1 Residual plots for ANOVA analysis for logarithm of diffOLS values

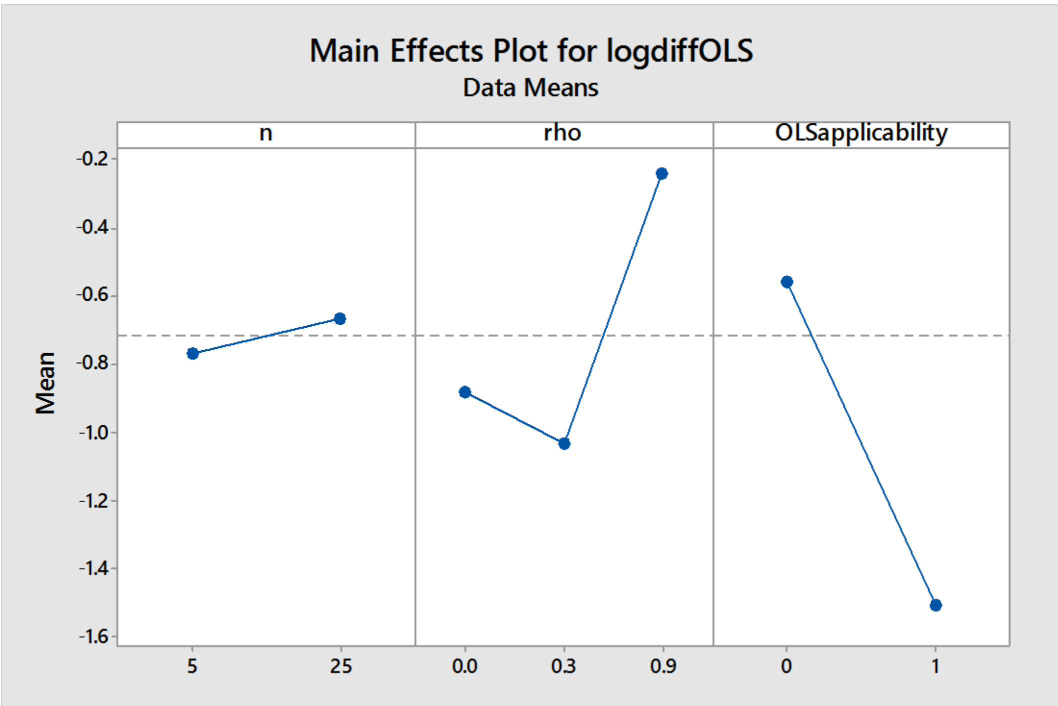

Figure E.2 Main effects plots for logarithm of diffOLS values

Table E.3 Result of ANOVA analysis for diffWLS values

General Linear Model: diffWLS versus n, rho, heteroscedas, set of predi, position of , ...

```
Method

Factor coding  (-1, 0, +1)

Stepwise Selection of Terms

α to enter = 0.15, α to remove = 0.15

Factor Information

Factor                        Type   Levels  Values
n                             Fixed       2  5, 25
heteroscedasticity            Fixed       2  0, 1
position of the design point  Fixed       2  0, 1

Analysis of Variance

Source                          DF   Adj SS    Adj MS  F-Value  P-Value
  n                              1  0.15958  0.159577    16.94    0.001
  heteroscedasticity             1  0.08808  0.088075     9.35    0.006
  position of the design point   1  0.13605  0.136052    14.45    0.001
Error                           20  0.18836  0.009418
Total                           23  0.57207

Model Summary

        S    R-sq  R-sq(adj)  R-sq(pred)
0.0970471  67.07%     62.13%      37.27%


Coefficients

Term                             Coef  SE Coef  T-Value  P-Value   VIF
Constant                       0.6748   0.0266    25.39    0.000
n
  5                           -0.0815   0.0198    -4.12    0.001  1.00
heteroscedasticity
  0                            0.0813   0.0266     3.06    0.006  1.00
position of the design point
  0                            0.0753   0.0198     3.80    0.001  1.00
```

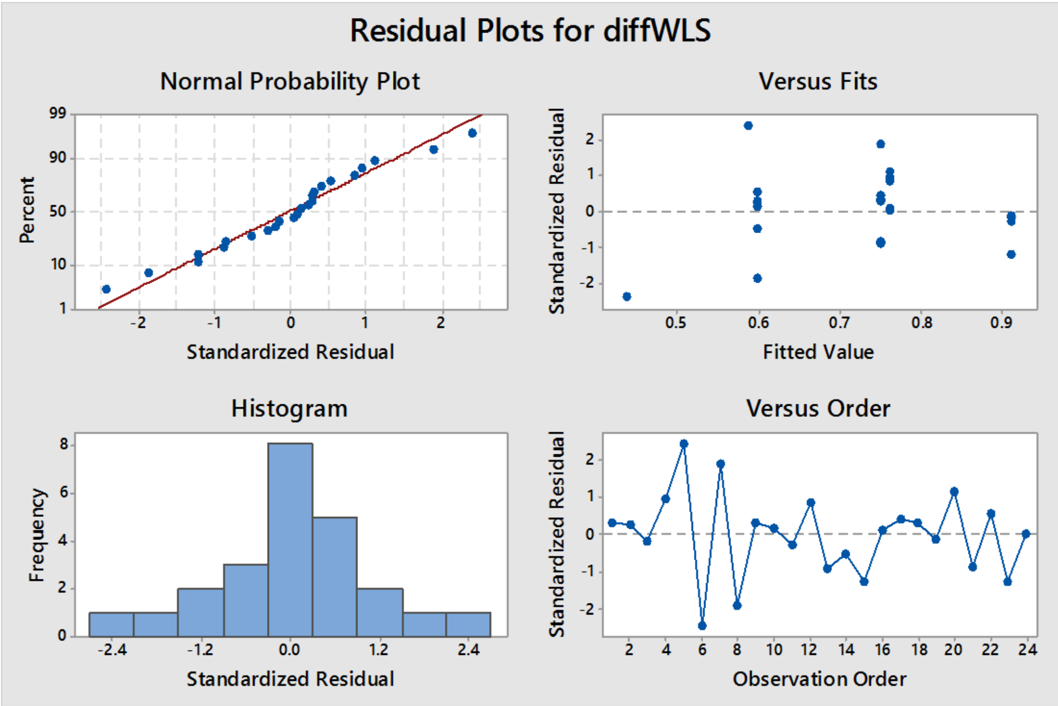

Figure E.3 Residual plots for ANOVA analysis for diffWLS values

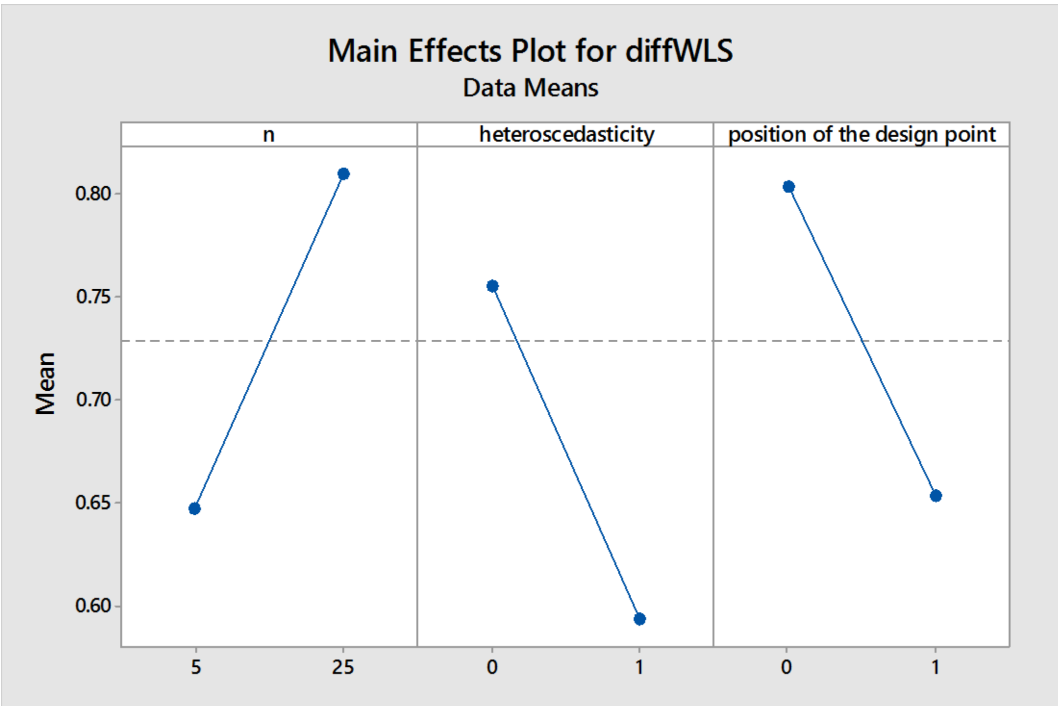

Figure E.4 Main effects plots for logarithm of diffWLS values

Table E.4 Result of ANOVA analysis for logarithm of diffSUR values

General Linear Model: logdiffSUR versus n, heteroscedasticity

```
Method

Factor coding  (-1, 0, +1)

Factor Information

Factor              Type   Levels  Values
n                   Fixed       2  5, 25
heteroscedasticity  Fixed       2  0, 1

Analysis of Variance

Source                DF  Adj SS   Adj MS  F-Value  P-Value
  n                    1  0.5062  0.50621    12.45    0.002
  heteroscedasticity   1  3.9327  3.93269    96.73    0.000
Error                 21  0.8538  0.04066
  Lack-of-Fit          1  0.1683  0.16828     4.91    0.038
  Pure Error          20  0.6855  0.03428
Total                 23  5.2927

Model Summary

       S    R-sq  R-sq(adj)  R-sq(pred)
0.201634  83.87%     82.33%      76.91%

Coefficients

Term                   Coef  SE Coef  T-Value  P-Value   VIF
Constant            -0.7834   0.0552   -14.19    0.000
n
  5                  0.1452   0.0412     3.53    0.002  1.00
heteroscedasticity
  0                 -0.5431   0.0552    -9.84    0.000  1.00
```

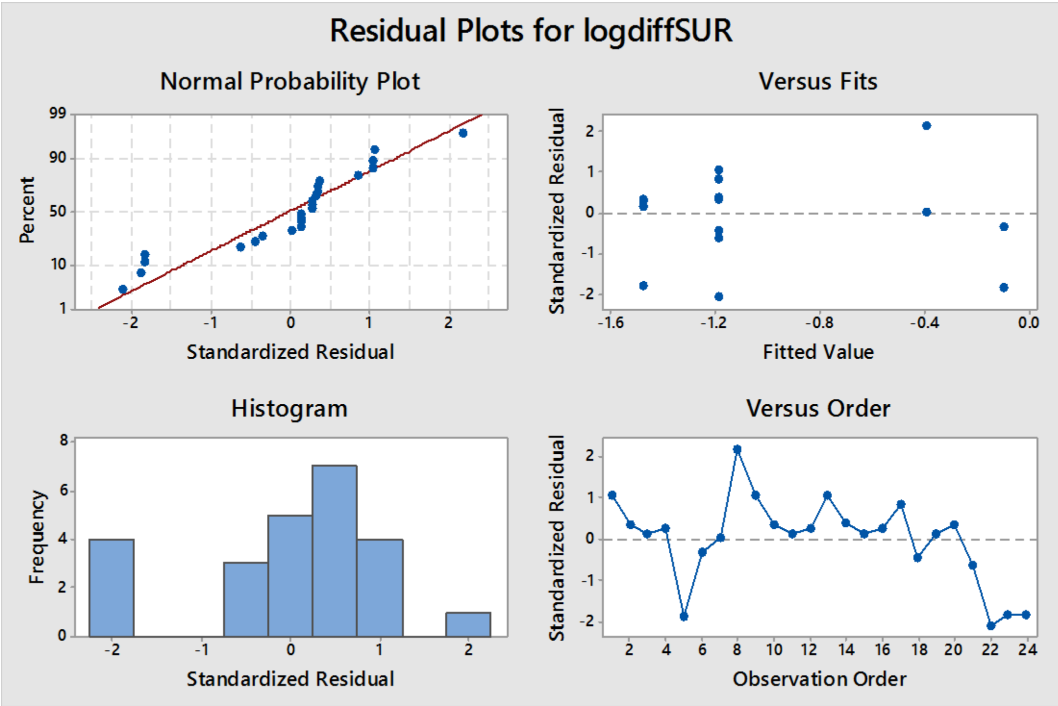

Figure E.5 Residual plots for ANOVA analysis for logarithm of diffSUR values

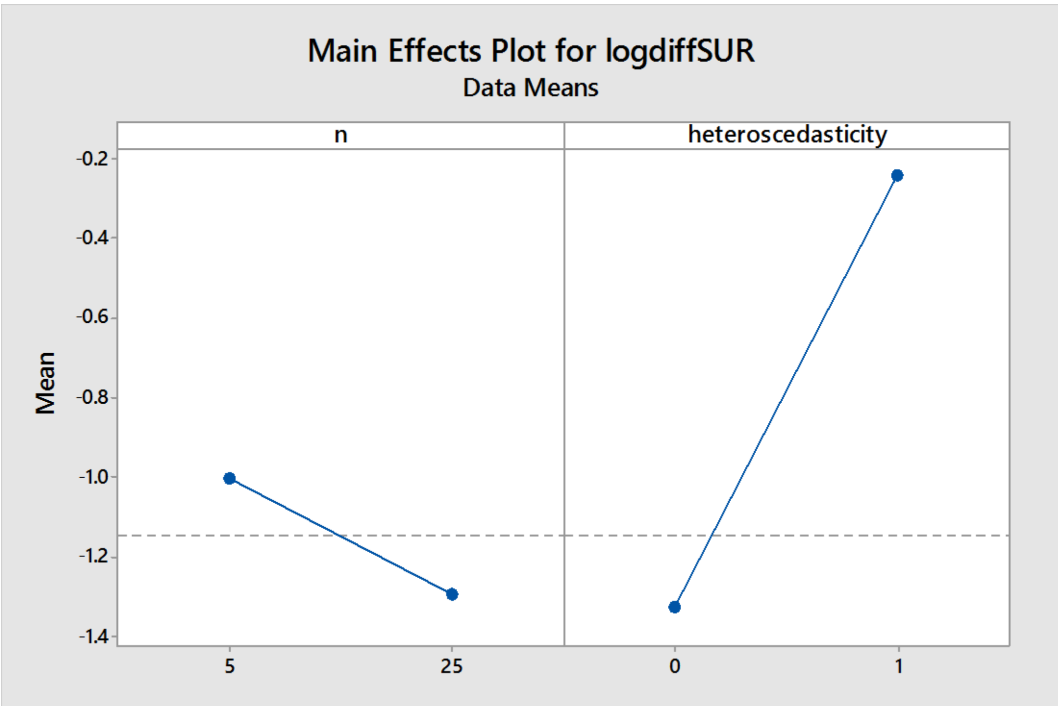

Figure E.6 Main effects plots for logarithm of diffSUR values